[redacted] type; shd be 10/517754
confirmed with Ross Shyge

```
=> file hcaplus
FILE 'HCAPLUS' ENTERED AT 16:20:47 ON 16 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 16 Apr 2007  VOL 146 ISS 17
FILE LAST UPDATED: 15 Apr 2007  (20070415/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos l16
L13          373 SEA FILE=HCAPLUS ABB=ON  PLU=ON  DOHERTY J?/AU
L14          912 SEA FILE=HCAPLUS ABB=ON  PLU=ON  NATARAJAN S?/AU
L15           52 SEA FILE=HCAPLUS ABB=ON  PLU=ON  STELMACH J?/AU
L16            4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L13 AND L14 AND L15
```

Inventor Search

```
=> d ibib ed abs l16 1-4

L16  ANSWER 1 OF 4  HCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2003:991289  HCAPLUS  Full-text
DOCUMENT NUMBER:          140:23240
TITLE:                    (Halo-benzo carbonyl)heterobicyclic p38 kinase
                          inhibiting agents
INVENTOR(S):              Doherty, James B.; Natarajan,
                          Swaminathan R.; Stelmach, John E.
PATENT ASSIGNEE(S):       Merck & Co., Inc., USA
SOURCE:                   PCT Int. Appl., 44 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------
     --------
     WO 2003103590         A2    20031218    WO 2003-US17821
                                                                     200306
                                                                     06
     WO 2003103590         A3    20040805
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI,
             NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ,
             TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
```

IN THE RE FORMAT

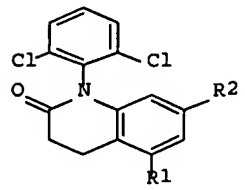
L16 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:943601 HCAPLUS Full-text
DOCUMENT NUMBER: 139:46382
TITLE: p38 MAP kinase inhibitors. Part 1: design and development of a new class of potent and highly selective inhibitors based on 3,4-dihydropyrido[3,2-d]pyrimidone scaffold
AUTHOR(S): **Natarajan, Swaminathan R.**; Wisnoski, David D.; Singh, Suresh B.; **Stelmach, John E.**; O'Neill, Edward A.; Schwartz, Cheryl D.; Thompson, Chris M.; Fitzgerald, Catherine E.; O'Keefe, Stephen J.; Kumar, Sanjeev; Hop, Cornelis E. C. A.; Zaller, Dennis M.; Schmatz, Dennis M.; **Doherty, James B.**
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(2), 273-276
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:46382
ED Entered STN: 13 Dec 2002
AB A new class of p38 antagonists based on 3,4-dihydropyrido[3,2,- d]pyrimidine scaffold has been developed. These inhibitors exhibit unprecedented selectivity towards p38 over other very closely related kinases. Three compds. were identified as benchmark analogs for follow-up studies. They show good potency for enzyme inhibition and excellent functional activity.
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L16 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:574925 HCAPLUS Full-text
DOCUMENT NUMBER: 137:140442
TITLE: Preparation of 1,5-diaryl-7-heterocyclyl(alkyl)-2-quinolinones as p38 protein kinase inhibitors
INVENTOR(S): **Doherty, James B.**; **Stelmach, John E.**; Chen, Meng-Hsin; Liu, Luping; Hunt, Julianne A.; Ruzek, Rowena D.; Goulet, Joung L.; Wisnoski, David D.; **Natarajan, Swaminathan Ravi**; Rupprecht, Kathleen M.; Bao, Jianming; Miao, Shouwu; Hong, Xingfang
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 440 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002058695	A1	20020801	WO 2001-US48676	200112 14
WO 2002058695	A9	20030912		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW

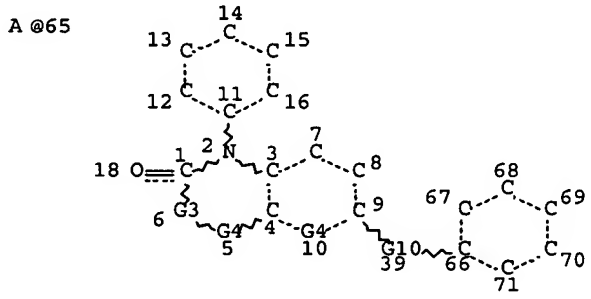
```
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
            BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI,
            FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG,
            CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
    CA 2431904          A1    20020801    CA 2001-2431904
                                                          200112
                                                          14
    AU 2002246677       A1    20020806    AU 2002-246677
                                                          200112
                                                          14
    EP 1345603          A1    20030924    EP 2001-994260
                                                          200112
                                                          14
        R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC,
            PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
    JP 2004521892       T     20040722    JP 2002-559029
                                                          200112
                                                          14
    US 2003092712       A1    20030515    US 2001-23231
                                                          200112
                                                          17
    US 6809199          B2    20041026
PRIORITY APPLN. INFO.:                    US 2000-256822P     P
                                                          200012
                                                          20

                                          WO 2001-US48676     W
                                                          200112
                                                          14

OTHER SOURCE(S):        MARPAT 137:140442
ED   Entered STN:  02 Aug 2002
GI
```



I

```
AB    Title compds. were prepared  Thus, 2,6-dibromo-4-methoxytoluene was converted in 5
      steps to arylquinolinone I (R1 = Br, R2 = OMe) which was condensed with 2,4-
      F2C6H3B(OH)2 and the O-demethylated product converted in 4 steps to I (R1 = C6H3F2-2,4,
      R2 = 4-piperidinyl). Data for biol. activity of title compds. were given.
REFERENCE COUNT:          1     THERE ARE 1 CITED REFERENCES AVAILABLE FOR
                                THIS RECORD. ALL CITATIONS AVAILABLE IN
                                THE RE FORMAT


=> d his nofile

     (FILE 'HOME' ENTERED AT 10:06:25 ON 16 APR 2007)

     FILE 'REGISTRY' ENTERED AT 10:06:38 ON 16 APR 2007
L7              STRUCTURE
L8            3 SEA SSS SAM L7
L9          112 SEA SSS FUL L7
                SAV L9 JAI754/A

     FILE 'HCAPLUS' ENTERED AT 13:42:12 ON 16 APR 2007
```

```
L10          22 SEA ABB=ON  PLU=ON  L9
L13         373 SEA ABB=ON  PLU=ON  DOHERTY J?/AU
L14         912 SEA ABB=ON  PLU=ON  NATARAJAN S?/AU
L15          52 SEA ABB=ON  PLU=ON  STELMACH J?/AU
L16           4 SEA ABB=ON  PLU=ON  L13 AND L14 AND L15
L17          19 SEA ABB=ON  PLU=ON  L10 NOT L16

     FILE 'HCAPLUS' ENTERED AT 16:20:47 ON 16 APR 2007
               D QUE NOS L16
               D IBIB ED ABS L16 1-4

=> file reg
FILE 'REGISTRY' ENTERED AT 16:21:36 ON 16 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   15 APR 2007  HIGHEST RN 930272-82-5
DICTIONARY FILE UPDATES:  15 APR 2007  HIGHEST RN 930272-82-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html


=> d stat que l9
L7                STR
```

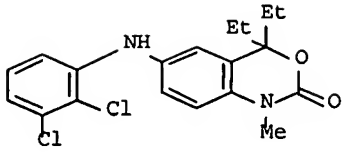



```
VAR G3=N/O/C
VAR G4=C/N
REP G10=(0-7) 65
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT  65
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   8
NUMBER OF NODES IS  25
```

```
STEREO ATTRIBUTES: NONE
L9             112 SEA FILE=REGISTRY SSS FUL L7

100.0% PROCESSED   49295 ITERATIONS                          112 ANSWERS
SEARCH TIME: 00.00.01


=> file hcaplus
FILE 'HCAPLUS' ENTERED AT 16:22:36 ON 16 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
the American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 16 Apr 2007  VOL 146 ISS 17
FILE LAST UPDATED: 15 Apr 2007  (20070415/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d que nos l10
L7                STR
L9            112 SEA FILE=REGISTRY SSS FUL L7
L10            22 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L9
```

Structure Search

```
=> d ibib abs hitstr l10 1-22

L10  ANSWER 1 OF 22  HCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2007:2702  HCAPLUS  Full-text
DOCUMENT NUMBER:          146:265786
TITLE:                    SAR studies of 6-(arylamino)-4,4-disubstituted-1-
                          methyl-1,4-dihydro-benzo[d][1,3]oxazin-2-ones as
                          progesterone receptor antagonists
AUTHOR(S):                Kern, Jeffrey C.; Terefenko, Eugene A.; Fensome,
                          Andrew; Unwallla, Ray; Wrobel, Jay; Zhu, Yuan;
                          Cohen, Jeffrey; Winneker, Richard; Zhang,
                          Zhiming; Zhang, Puwen
CORPORATE SOURCE:         Chemical and Screening Sciences, Wyeth Research,
                          Collegeville, PA, 19426, USA
SOURCE:                   Bioorganic & Medicinal Chemistry Letters (2007),
                          17(1), 189-192
                          CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER:                Elsevier Ltd.
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
GI
```



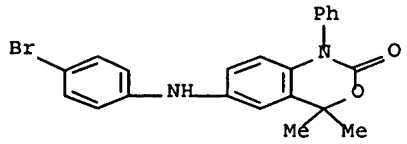
I

AB We previously disclosed that 6-aryl benzoxazin-2-ones were PR modulators. In a continuation of this work we examined the SAR of new 6-arylamino benzoxazinones and found the targets 1-25, with an extra amino linker between the pendent 6-aryl groups and benzoxazinone or benzoxazine-2-thione core, were PR antagonists. A series of compds. with substituents at the 1- and 4-positions as well as different 6-aryl groups were prepared and tested in the T47D cell alkaline phosphatase assay. Interestingly, the SAR unveiled from the 6-arylamino benzoxazinones was quite different from those of their parent compds. For example, in contrast to the 6-aryl benzoxazinones, Me substitution at the 1-position significantly increased the potency of 6-arylamino benzoxazinones. Several 6-arylamino benzoxazinones (e.g., 12 (I), IC50 = 5.0 nM) had low nanomolar in vitro potency as PR antagonists in the T47D cell alkaline phosphatase assay.

IT **926691-71-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(arylamino benzoxazinones as progesterone receptor antagonists)

RN 926691-71-6 HCAPLUS

CN 2H-3,1-Benzoxazin-2-one, 6-[(4-bromophenyl)amino]-1,4-dihydro-4,4-dimethyl-1-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:588645 HCAPLUS Full-text

DOCUMENT NUMBER: 143:115550

TITLE: Preparation of heterocyclic compounds as selective norepinephrine reuptake inhibitors for treating hot flashes, impulse control disorders and personality change due to a general medical condition

INVENTOR(S): Allen, Albert John; Hemrick-Luecke, Susan; Sumner, Calvin Russell; Wallace, Owen Brendan

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: PCT Int. Appl., 337 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

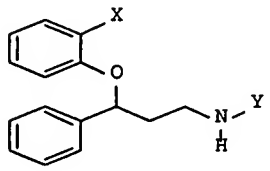
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

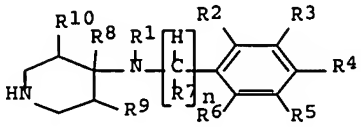
WO 2005060949	A2	20050707	WO 2004-US38221 200412 01
WO 2005060949	A3	20050909	
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW		
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG		
CA 2548304	A1	20050707	CA 2004-2548304 200412 01
EP 1729754	A2	20061213	EP 2004-811076 200412 01
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR		
CN 1889940	A	20070103	CN 2004-80036841 200412 01
US 2007015786	A1	20070118	US 2006-581015 200605 30
PRIORITY APPLN. INFO.:			US 2003-529428P P 200312 12
			WO 2004-US38221 W 200412 01

OTHER SOURCE(S): MARPAT 143:115550

GI



I



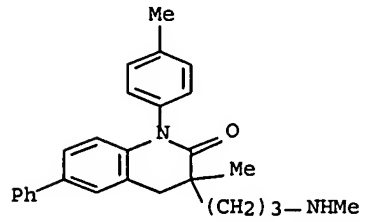
II

AB The invention relates to a method of preventing or treating hot flashes, vasomotor symptoms, impulse control disorders or personality change due to a general medical condition, comprising administering to a patient in need thereof a therapeutically effective amount of a selective norepinephrine reuptake inhibitor selected from atomoxetine, reboxetine, I [X = alkylthio; Y = alkyl], II [n = 1-3; R1 = alkyl, alkenyl, cycloalkyl, etc.; R2-R4 = H, alkyl, alkoxy, etc.; R5-R6 = H, alkyl, alkoxy, halo; R7-R8 = H, alkyl; R9-R10 = H, halo, OH, CN, alkyl, alkoxy], etc. Over 200 title compds. such as I, II and other heterocyclic compds. disclosed, were prepared E.g., a 2-step synthesis of N-(2-methylpropyl)-N-[(2-fluorophenyl)methyl]piperidin-4-amine fumarate, starting from tert-Bu 4-(2-methylpropylamino)piperidine-1- carboxylate and 2-fluorobenzaldehyde, was given. The preferred exemplified title compds. exhibit a Ki

value less than 1 μM, more preferably less than 500 nM at the norepinephrine transporter as determined using the scintillation proximity assay.

IT 792122-61-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic compds. as selective norepinephrine reuptake inhibitors for treating hot flashes, impulse control disorders and personality change due to general medical condition)

RN 792122-61-3 HCAPLUS
CN 2(1H)-Quinolinone, 3,4-dihydro-3-methyl-3-[3-(methylamino)propyl]-1-(4-methylphenyl)-6-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 3 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:523264 HCAPLUS Full-text
DOCUMENT NUMBER: 143:59831
TITLE: A preparation of aminopiperidine derivatives, useful for the treatment of cognitive failure
INVENTOR(S): Hatfield, Alan Kramer; Bymaster, Franklin Porter; McKinzie, David Lee; Tucker, Tina Marie; Keaffaber, Kirk Matthew; Sumner, Calvin Russell; Trzepacz, Paula Terese; Allen, Albert John; Kelsey, Douglas Kenneth; Michelson, David; Gehlert, Donald Richard; Yang, Charles Renkin
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 300 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005053663	A2	20050616	WO 2004-US37195	200411 24
WO 2005053663	A3	20050811		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

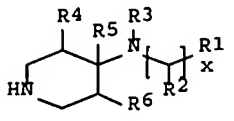
PRIORITY APPLN. INFO.: US 2003-524450P P

200311
24

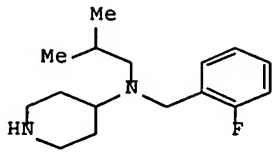
US 2003-524781P P

200311
25

OTHER SOURCE(S): MARPAT 143:59831
GI



I



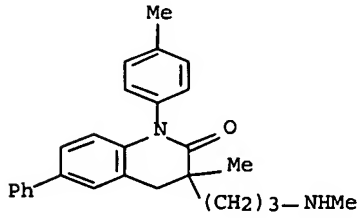
II

AB The invention relates to a preparation of aminopiperidine derivs. of formula I [wherein: x is 1-3; R1 is (un)substituted phenyl; R2 and R5 are independently H or alkyl; R3 is (cyclo)alkyl, alkenyl, or cycloalkylalkyl, etc.; R4 is H, halogen, or OH, etc.; R6 is H, halogen, CN, or alkyl, etc.], useful for the treatment of cognitive failure. Selective norepinephrine reuptake inhibitors were used to treat cognitive failure. For instance, fumarate salt of aminopiperidine derivative II was prepared via imination of 2-fluorobenzaldehyde by tert-Bu 4-[(2-methylpropyl)amino]piperidine- 1-carboxylate, reduction of the obtained imine, and subsequent fumaric acid salt formation. The preferred invention compds. exhibit Ki values less than 500 nM at the norepinephrine transporter.

IT **792122-61-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aminopiperidine derivs. useful for the treatment of cognitive failure)

RN 792122-61-3 HCAPLUS

CN 2(1H)-Quinolinone, 3,4-dihydro-3-methyl-3-[3-(methylamino)propyl]-1-(4-methylphenyl)-6-phenyl- (9CI) (CA INDEX NAME)



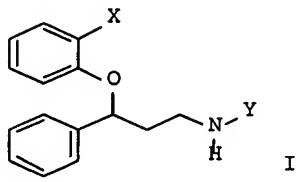
L10 ANSWER 4 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:216719 HCAPLUS Full-text
DOCUMENT NUMBER: 142:291416
TITLE: Treatment of stuttering and other communication disorders with norepinephrine reuptake inhibitors
INVENTOR(S): Kelsey, Douglas Kenneth
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 299 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

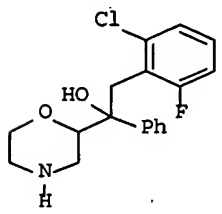
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005021095	A2	20050310	WO 2004-US25591	20040825
WO 2005021095	A3	20050609		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2532349	A1	20050310	CA 2004-2532349	20040825
EP 1660185	A2	20060531	EP 2004-780429	20040825
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
US 2007032554	A1	20070208	US 2006-568269	20060214
PRIORITY APPLN. INFO.:			US 2003-498018P P	20030827
			WO 2004-US25591 W	20040825

OTHER SOURCE(S): MARPAT 142:291416

GI



I



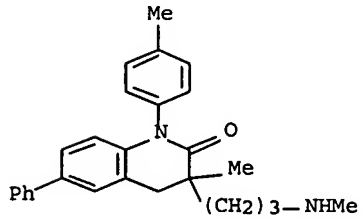
II

AB Provided are methods and medicaments for treating stuttering or another communication disorder, comprising administering to a patient in need of such treatment an effective amount of a selective norepinephrine reuptake inhibitor. The invention discloses the use of atomoxetine, racemic reboxetine, (S,S)-reboxetine, and compds. of formula I [wherein X = alkylthio and Y = alkyl; as described in U.S. patent Number 5,281,624], as well as their pharmaceutically acceptable salts, as the norepinephrine reuptake inhibitors described for treatment purposes. The invention further discloses the preparation of addnl. heterocyclic derivs. (as well as their pharmaceutically acceptable salts) that possess ability to serve as norepinephrine reuptake inhibitors. For instance, morpholine derivative II•HCl was prepared via alkylation of (4-benzyl-morpholin-2-yl)(phenyl)methanone with 2-chloro-6-fluorobenzylmagnesium chloride and subsequent N-debenzylation. The preferred invention compds. exhibited Ki values of less than 500 nM at the norepinephrine transporter (scintillation proximity assay).

IT **792122-61-3P**, 3-Methyl-3-(3-methylamino-propyl)-6-phenyl-1-p-tolyl-3,4-dihydro-1H-quinolin-2-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic compds. useful as norepinephrine reuptake inhibitors)

RN 792122-61-3 HCAPLUS

CN 2(1H)-Quinolinone, 3,4-dihydro-3-methyl-3-[3-(methylamino)propyl]-1-(4-methylphenyl)-6-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 5 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:216660 HCAPLUS Full-text
DOCUMENT NUMBER: 142:291415
TITLE: Treatment of pervasive development disorders employing norepinephrine reuptake inhibitors
INVENTOR(S): Allen, Albert John; Kelsey, Douglas Kenneth
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 300 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005020976	A2	20050310	WO 2004-US25593	20040825
WO 2005020976	A3	20050616		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW,

AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ,
DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL,
PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ,
GW, ML, MR, NE, SN, TD, TG

CA 2536161	A1	20050310	CA 2004-2536161	200408 25
EP 1660065	A2	20060531	EP 2004-780431	200408 25
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
US 2006241188	A1	20061026	US 2006-568466	200602 14

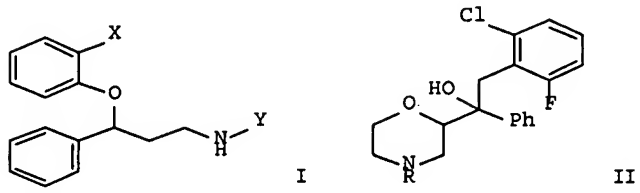
PRIORITY APPLN. INFO.:

US 2003-498146P P 200308 27

WO 2004-US25593 W 200408 25

OTHER SOURCE(S): MARPAT 142:291415

GI



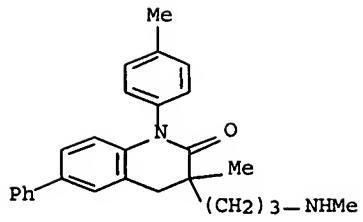
I II

AB Provided are methods and medicaments for treating a pervasive development disorder, comprising administering to a patient in need of such treatment an effective amount of a selective norepinephrine reuptake inhibitor. The invention discloses the use of atomoxetine, racemic reboxetine, (S,S)-reboxetine, and compds. of formula I [wherein X = alkylthio and Y = alkyl; as described in U.S. patent Number 5,281,624], as well as their pharmaceutically acceptable salts, as the norepinephrine reuptake inhibitors described for treatment purposes. The invention further discloses the preparation of addnl. heterocyclic derivs. (as well as their pharmaceutically acceptable salts) that possess ability to serve as norepinephrine reuptake inhibitors. For instance, morpholine derivative II•HCl (R = H) was prepared via alkylation of (4-benzyl-morpholin-2-yl)(phenyl)methanone by 2-chloro-6-fluorobenzylmagnesium chloride and subsequent N-debenzylation of the obtained alc. I (R = Bn). The preferred invention compds. exhibited Ki values of less than 500 nM at the norepinephrine transporter (scintillation proximity assay).

IT **792122-61-3P**, 3-Methyl-3-(3-methylamino-propyl)-6-phenyl-1-p-tolyl-3,4-dihydro-1H-quinolin-2-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic compds. useful as norepinephrine reuptake inhibitors)

RN 792122-61-3 HCAPLUS

CN 2(1H)-Quinolinone, 3,4-dihydro-3-methyl-3-[3-(methylamino)propyl]-1-(4-methylphenyl)-6-phenyl- (9CI) (CA INDEX NAME)

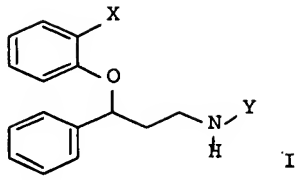


L10 ANSWER 6 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:216659 HCAPLUS Full-text
DOCUMENT NUMBER: 142:291414
TITLE: Treatment of learning disabilities and motor skills disorder with norepinephrine reuptake inhibitors
INVENTOR(S): Sumner, Calvin Russell
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 304 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

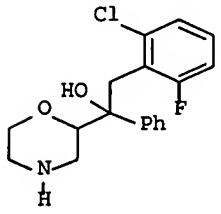
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005020975	A2	20050310	WO 2004-US25592	200408 25
WO 2005020975	A3	20050602		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2530014	A1	20050310	CA 2004-2530014	200408 25
EP 1660064	A2	20060531	EP 2004-780430	200408 25
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				

PRIORITY APPLN. INFO.:
US 2003-498019P P 200308 27
WO 2004-US25592 W 200408 25

OTHER SOURCE(S): MARPAT 142:291414
GI



I



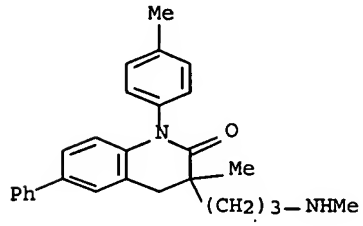
II

AB Provided are methods and medicaments for treating a learning disability or a motor skills disorder, comprising administering to a patient in need of such treatment an effective amount of a selective norepinephrine reuptake inhibitor. The invention discloses the use of atomoxetine, racemic reboxetine, (S,S)-reboxetine, and compds. of formula I [wherein X = alkylthio and Y = alkyl; as described in U.S. patent Number 5,281,624], as well as their pharmaceutically acceptable salts, as the norepinephrine reuptake inhibitors described for treatment purposes. The invention further discloses the preparation of addnl. heterocyclic derivs. (as well as their pharmaceutically acceptable salts) that possess ability to serve as norepinephrine reuptake inhibitors. For instance, morpholine derivative II•HCl was prepared via alkylation of (4-benzyl-morpholin-2-yl)(phenyl)methanone with 2-chloro-6-fluorobenzylmagnesium chloride and subsequent N-debenzylation. The preferred invention compds. exhibited Ki values of less than 500 nM at the norepinephrine transporter (scintillation proximity assay).

IT **792122-61-3P**, 3-Methyl-3-(3-methylamino-propyl)-6-phenyl-1-p-tolyl-3,4-dihydro-1H-quinolin-2-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic compds. useful as norepinephrine reuptake inhibitors)

RN 792122-61-3 HCAPLUS

CN 2(1H)-Quinolinone, 3,4-dihydro-3-methyl-3-[3-(methylamino)propyl]-1-(4-methylphenyl)-6-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 7 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1072170 HCAPLUS Full-text
DOCUMENT NUMBER: 142:190226
TITLE: Interaction Profiles of Protein Kinase-Inhibitor Complexes and Their Application to Virtual Screening

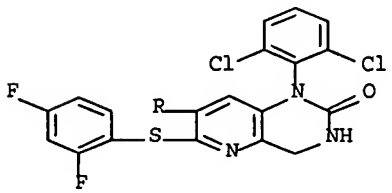
AUTHOR(S): Chuaqui, Claudio; Deng, Zhan; Singh, Juswinder
CORPORATE SOURCE: Computational Drug Design Group, Department of Research Informatics, Biogen Idec, Inc., Cambridge, MA, 01242, USA
SOURCE: Journal of Medicinal Chemistry (2005), 48(1), 121-133
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

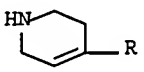
AB A major challenge facing structure-based drug discovery efforts is how to leverage the massive amount of exptl. (x-ray and NMR) and virtual structural information generated from drug discovery projects. Many important drug targets have large nos. of protein-inhibitor complexes, necessitating tools to compare and contrast their similarities and differences. This information would be valuable for understanding potency and selectivity of inhibitors and could be used to define target constraints to assist virtual screening. The authors describe a profile-based approach that enables us to capture the conservation of interactions between a set of protein-ligand receptor complexes. The use of profiles provides a sensitive means to compare multiple inhibitors binding to a drug target. The authors demonstrate the utility of profile-based anal. of small mol. complexes from the protein-kinase family to identify similarities and differences in binding of ATP, p38, and CDK2 compds. to kinases and how these profiles can be applied to differentiate the selectivity of these inhibitors. Importantly, our virtual screening results demonstrate superior enrichment of kinase inhibitors using profile-based methods relative to traditional scoring functions. Interaction-based anal. should provide a valuable tool for understanding inhibitor binding to other important drug targets.

IT **616894-42-9**
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(interaction profiles of protein kinase-inhibitor complexes and their application to virtual screening)

RN 616894-42-9 HCAPLUS

CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-(1,2,3,6-tetrahydro-4-pyridinyl)-(9CI) (CA INDEX NAME)





REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 8 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:1036891 HCAPLUS Full-text
DOCUMENT NUMBER: 142:16841
TITLE: Treatment of emotional dysregulation
INVENTOR(S): Allen, Albert John; Cloutier, Kathleen Ann; Michelson, David; Reimherr, Frederick William
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 155 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004103356	A2	20041202	WO 2004-US13005	200405 11
WO 2004103356	A3	20050331		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-470752P P 200305 15

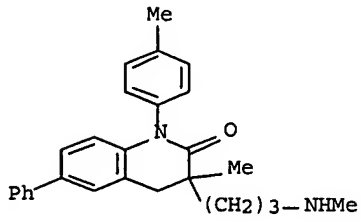
OTHER SOURCE(S): MARPAT 142:16841

AB Provided is a method of treating emotional dysregulation comprising administering to a patient in need of such treatment a selective norepinephrine reuptake inhibitor.

IT **792122-61-3P**, 3-Methyl-3-(3-methylaminopropyl)-6-phenyl-1-p-tolyl-3,4-dihydro-1H-quinolin-2-one
RL: SPN (Synthetic preparation); PREP (Preparation)
(treatment of emotional dysregulation)

RN 792122-61-3 HCAPLUS

CN 2(1H)-Quinolinone, 3,4-dihydro-3-methyl-3-[3-(methylamino)propyl]-1-(4-methylphenyl)-6-phenyl- (9CI) (CA INDEX NAME)



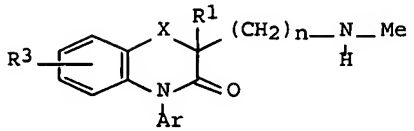
L10 ANSWER 9 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:965224 HCAPLUS Full-text
DOCUMENT NUMBER: 141:410824
TITLE: Quinolone derivatives useful as selective norepinephrine reuptake inhibitors, and their preparation, pharmaceutical compositions, and use in the treatment of nervous system disorders.
INVENTOR(S): Camp, Nicholas Paul; Penariol, Roberta; Beadle, Christopher David
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

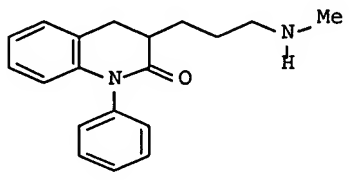
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004096773	A1	20041111	WO 2004-US9290	200404 16
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2518753	A1	20041111	CA 2004-2518753	200404 16
EP 1622874	A1	20060208	EP 2004-760215	200404 16
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
JP 2006524689	T	20061102	JP 2006-509339	200404 16

PRIORITY APPLN. INFO.:	GB 2003-9440	A	200304 25
	US 2003-477277P	P	200306 10
	WO 2004-US9290	W	200404 16

OTHER SOURCE(S): MARPAT 141:410824
GI



I



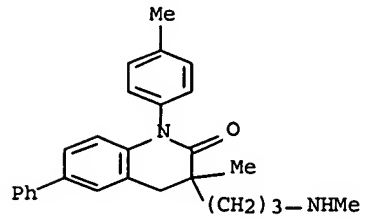
II

AB The invention relates to compds. I, and their preparation and use as selective norepinephrine reuptake inhibitors (no data). In formula I, X is C(R4R5), O, or S; n is 2 or 3; R1 is H or C1-C4 alkyl; R3 is H, halo, C1-C4 alkyl, O(C1-C4 alkyl), nitrile, Ph, or substituted Ph; R4 and R5 are each independently H or C1-C4 alkyl; Ar is optionally substituted Ph, furanyl, thienyl, or pyrrolyl (substituents include halo, Me, Et, trifluoromethyl, nitrile, methoxy, or fluoro, in specific positions); and includes pharmaceutically acceptable salts. The compds. are potentially useful for the treatment of a variety of nervous system disorders. Approx. 30 racemic compds. and several D-tartrate salts of unspecified enantiomers were prepared For example, 3,4-dihydro-1H-quinolin-2-one was N-arylated by PhBr in the presence of CuI, K2CO3, and trans-cyclohexane-1,2-diamine, followed by lithiation with LiHDMS, alkylation with Br(CH2)3Cl, and amination with MeNH2 in the presence of KI, to give title compound II.

IT **792122-61-3P**, 3-Methyl-3-(3-methylaminopropyl)-6-phenyl-1-p-tolyl-3,4-dihydro-1H-quinolin-2-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of [(methylamino)alkyl]quinolone derivs. as selective norepinephrine reuptake inhibitors for treatment of nervous system disorders)

RN 792122-61-3 HCAPLUS

CN 2(1H)-Quinolinone, 3,4-dihydro-3-methyl-3-[3-(methylamino)propyl]-1-(4-methylphenyl)-6-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 10 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:1001966 HCAPLUS Full-text

DOCUMENT NUMBER: 140:321317

TITLE: A novel Pd-catalyzed cyclization reaction of ureas for the synthesis of dihydroquinazolinone p38 kinase inhibitors

AUTHOR(S): Schlapbach, Achim; Heng, Richard; Di Padova, Franco

CORPORATE SOURCE: Novartis Institute for Biomedical Research, Arthritis and Bone Metabolism, Basel, CH-4002, Switz.

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(2), 357-360
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:321317

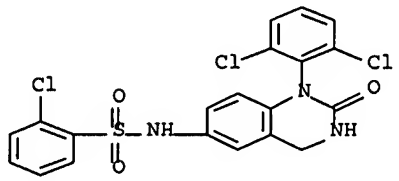
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

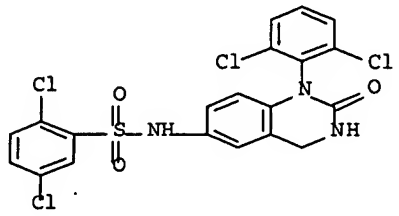
AB A series of potent p38 inhibitors based on the dihydroquinazoline scaffold was synthesized using a novel Pd-catalyzed cyclization reaction of aryl benzyl ureas. For example, cyclization of a urea derivative (I) gave 1-(4-hydroxy-2,6-dimethylphenyl)-3,4-dihydro-6-nitro- 2(1H)-quinazolinone (II). Sequential treatment of II with 4-(3-chloropropyl)morpholine and then with 3-chloro-4- fluorobenzenesulfonyl chloride a 2(1H)-quinazolinone derivative (III). Optimization of this compound class led to III, which inhibits p38α in vitro with IC50 = 14 nM and is active in the mouse TNFα-release model.

IT **678173-09-6 678173-10-9 678173-11-0**
678173-12-1 678173-13-2 678173-14-3
RL: PAC (Pharmacological activity); BIOL (Biological study)
(preparation of dihydro-2(1H)-quinazolinone derivs. by palladium-catalyzed cyclization of urea derivs. and their study as p38 kinase inhibitors and TNFα release inhibitors)

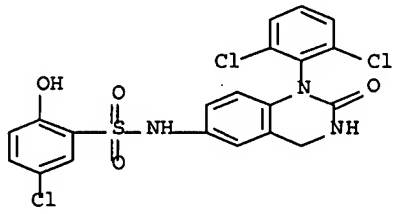
RN 678173-09-6 HCAPLUS
CN Benzenesulfonamide, 2-chloro-N-[1-(2,6-dichlorophenyl)-1,2,3,4-tetrahydro-2-oxo-6-quinazolinyl]- (9CI) (CA INDEX NAME)



RN 678173-10-9 HCAPLUS
CN Benzenesulfonamide, 2,5-dichloro-N-[1-(2,6-dichlorophenyl)-1,2,3,4-tetrahydro-2-oxo-6-quinazolinyl]- (9CI) (CA INDEX NAME)

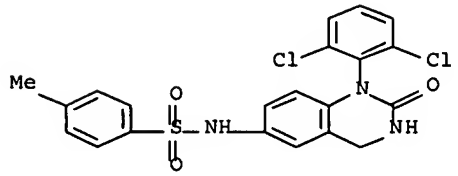


RN 678173-11-0 HCAPLUS
CN Benzenesulfonamide, 5-chloro-N-[1-(2,6-dichlorophenyl)-1,2,3,4-tetrahydro-2-oxo-6-quinazolinyl]-2-hydroxy- (9CI) (CA INDEX NAME)

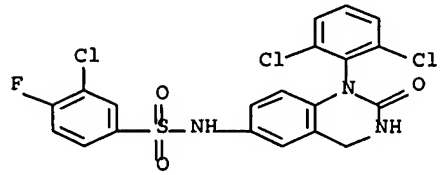


RN 678173-12-1 HCAPLUS
CN Benzenesulfonamide, N-[1-(2,6-dichlorophenyl)-1,2,3,4-tetrahydro-2-

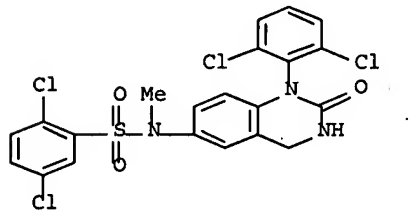
oxo-6-quinazolinyl]-4-methyl- (9CI) (CA INDEX NAME)



RN 678173-13-2 HCAPLUS
CN Benzenesulfonamide, 3-chloro-N-[1-(2,6-dichlorophenyl)-1,2,3,4-tetrahydro-2-oxo-6-quinazolinyl]-4-fluoro- (9CI) (CA INDEX NAME)

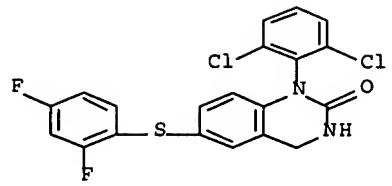


RN 678173-14-3 HCAPLUS
CN Benzenesulfonamide, 2,5-dichloro-N-[1-(2,6-dichlorophenyl)-1,2,3,4-tetrahydro-2-oxo-6-quinazolinyl]-N-methyl- (9CI) (CA INDEX NAME)

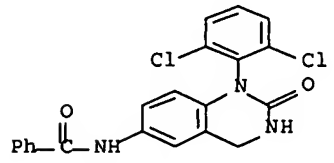


IT **252265-88-6P**, 1-(2,6-Dichlorophenyl)-6-[(2,4-difluorophenyl)sulfanyl]-3,4-dihydro-1H-quinazolin-2-one **678173-05-2P 678173-06-3P**, 1-(2,6-Dichlorophenyl)-6-[(2,4-difluorophenyl)amino]-3,4-dihydro-2(1H)-quinazolinone **678173-07-4P 678173-08-5P 678173-30-3P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of dihydro-2(1H)-quinazolinone derivs. by palladium-catalyzed cyclization of urea derivs. and their study as p38 kinase inhibitors and TNFα release inhibitors)

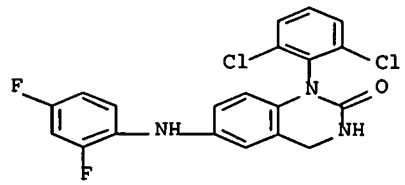
RN 252265-88-6 HCAPLUS
CN 2(1H)-Quinazolinone, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



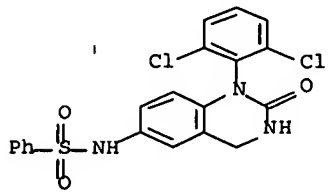
RN 678173-05-2 HCAPLUS
CN Benzamide, N-[1-(2,6-dichlorophenyl)-1,2,3,4-tetrahydro-2-oxo-6-quinazolinyl]- (9CI) (CA INDEX NAME)



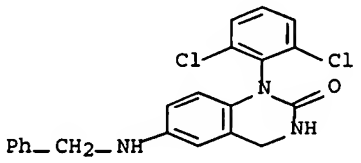
RN 678173-06-3 HCAPLUS
CN 2(1H)-Quinazolinone, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)amino]-3,4-dihydro- (9CI) (CA INDEX NAME)



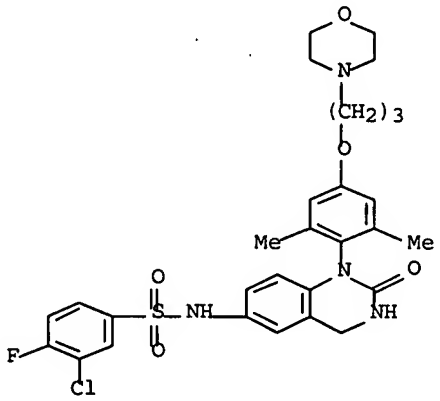
RN 678173-07-4 HCAPLUS
CN Benzenesulfonamide, N-[1-(2,6-dichlorophenyl)-1,2,3,4-tetrahydro-2-oxo-6-quinazolinyl]- (9CI) (CA INDEX NAME)



RN 678173-08-5 HCAPLUS
CN 2(1H)-Quinazolinone, 1-(2,6-dichlorophenyl)-3,4-dihydro-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 678173-30-3 HCAPLUS
CN Benzenesulfonamide, 3-chloro-N-[1-[2,6-dimethyl-4-[3-(4-morpholinyl)propoxy]phenyl]-1,2,3,4-tetrahydro-2-oxo-6-quinazolinyl]-4-fluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 11 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:991289 HCAPLUS Full-text
DOCUMENT NUMBER: 140:23240
TITLE: (Halo-benzo carbonyl)heterobicyclic p38 kinase inhibiting agents
INVENTOR(S): Doherty, James B.; Natarajan, Swaminathan R.; Stelmach, John E.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 44 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003103590	A2	20031218	WO 2003-US17821	20030606
WO 2003103590	A3	20040805		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2488567	A1	20031218	CA 2003-2488567	20030606
AU 2003238915	A1	20031222	AU 2003-238915	20030606
EP 1515727	A2	20050323	EP 2003-734435	20030606
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005176723	A1	20050811	US 2003-517754	20030606
JP 2005534649	T	20051117	JP 2004-510711	20030606
PRIORITY APPLN. INFO.:			US 2002-388066P P	20020611
			WO 2003-US17821 W	20030606

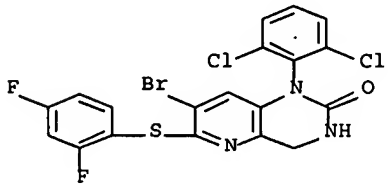
OTHER SOURCE(S): MARPAT 140:23240

AB Heterobicyclic compds. are claimed which are inhibitors of p38 and are useful in the treatment of inflammation such as in the treatment of rheumatoid arthritis, rheumatoid spondylitis, osteoarthritis, gouty arthritis and other arthritic conditions; inflamed joints, eczema, psoriasis or other inflammatory skin conditions such as sunburn; inflammatory eye conditions including conjunctivitis; pyresis, pain and other conditions associated with inflammation.

IT **547756-25-2P 632628-12-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(heterobicyclic p38 kinase inhibiting agents)

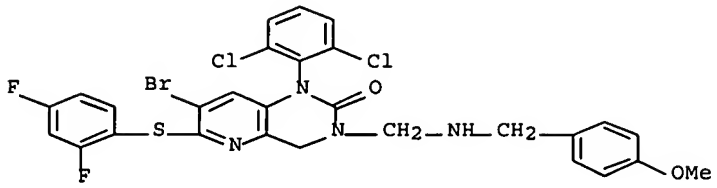
RN 547756-25-2 HCAPLUS

CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 7-bromo-1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



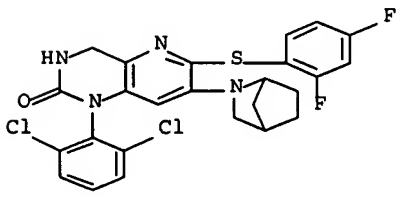
RN 632628-12-7 HCAPLUS

CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 7-bromo-1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-3-[[[(4-methoxyphenyl)methyl]amino]methyl]- (9CI) (CA INDEX NAME)

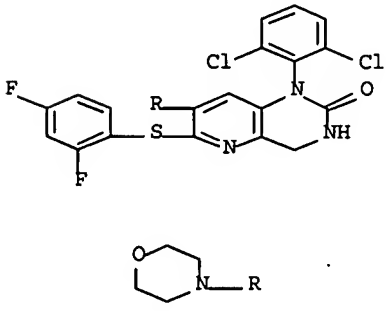


IT **547756-27-4P 547756-28-5P 547756-29-6P**
547756-30-9P 547756-32-1P 547756-34-3P
547756-35-4P 547756-36-5P 547756-44-5P
632628-13-8P 632628-14-9P 632628-15-0P
632628-16-1P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(heterobicyclic p38 kinase inhibiting agents)

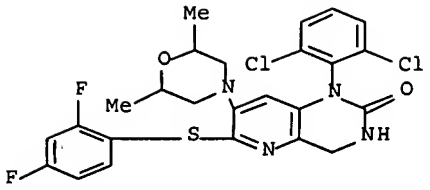
RN 547756-27-4 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 7-(2-azabicyclo[2.2.1]hept-2-yl)-1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



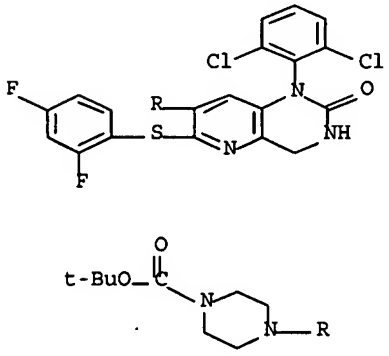
RN 547756-28-5 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-(4-morpholinyl)- (9CI) (CA INDEX NAME)



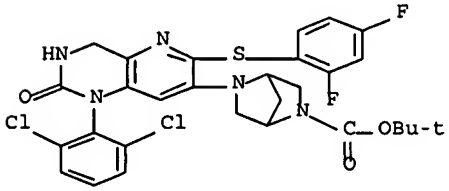
RN 547756-29-6 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-7-(2,6-dimethyl-4-morpholinyl)-3,4-dihydro- (9CI) (CA INDEX NAME)



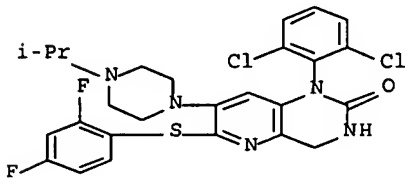
RN 547756-30-9 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-1,2,3,4-tetrahydro-2-oxopyrido[3,2-d]pyrimidin-7-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



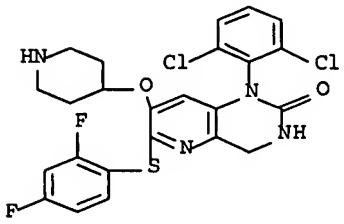
RN 547756-32-1 HCAPLUS
CN 2,5-Diazabicyclo[2.2.1]heptane-2-carboxylic acid, 5-[1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-1,2,3,4-tetrahydro-2-oxopyrido[3,2-d]pyrimidin-7-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



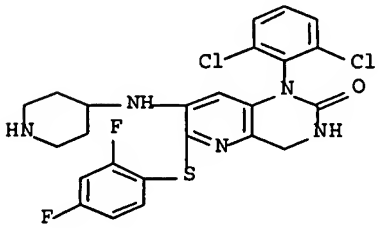
RN 547756-34-3 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-[4-(1-methylethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



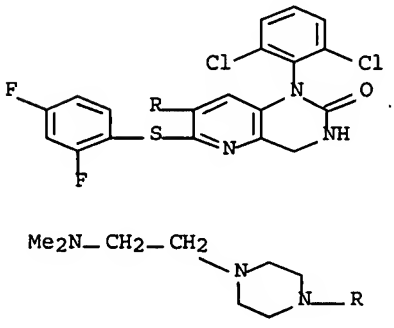
RN 547756-35-4 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-(4-piperidinyloxy)- (9CI) (CA INDEX NAME)



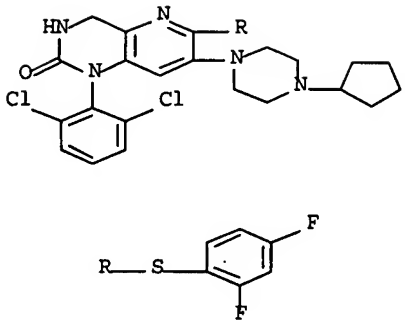
RN 547756-36-5 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-(4-piperidinylamino)- (9CI) (CA INDEX NAME)



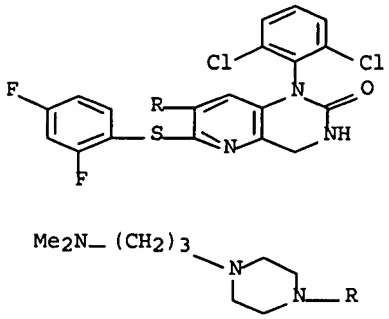
RN 547756-44-5 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-7-[4-[2-(dimethylamino)ethyl]-1-piperazinyl]-3,4-dihydro- (9CI) (CA INDEX NAME)



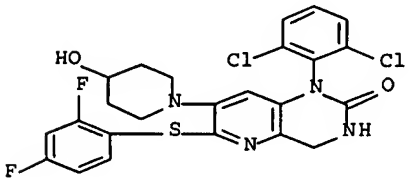
RN 632628-13-8 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 7-(4-cyclopentyl-1-piperazinyl)-1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



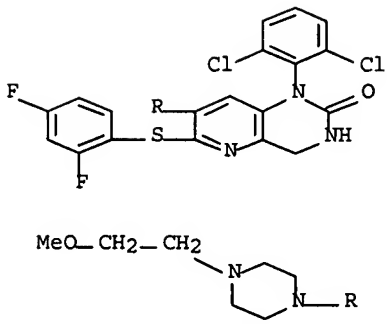
RN 632628-14-9 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-7-[4-[3-(dimethylamino)propyl]-1-piperazinyl]-3,4-dihydro- (9CI) (CA INDEX NAME)



RN 632628-15-0 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-(4-hydroxy-1-piperidinyl)- (9CI) (CA INDEX NAME)



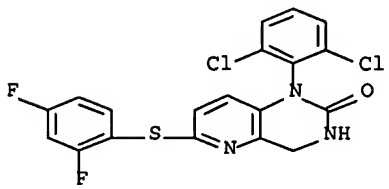
RN 632628-16-1 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-[4-(2-methoxyethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



L10 ANSWER 12 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:841822 HCAPLUS Full-text
DOCUMENT NUMBER: 140:87056
TITLE: SAR of 3,4-Dihydropyrido[3,2-d]pyrimidone p38 inhibitors
AUTHOR(S): Liu, Luping; Stelmach, John E.; Natarajan, Swaminathan R.; Chen, Meng-Hsin; Singh, Suresh B.; Schwartz, Cheryl D.; Fitzgerald, Catherine E.; O'Keefe, Stephen J.; Zaller, Dennis M.; Schmatz, Dennis M.; Doherty, James B.
CORPORATE SOURCE: Departments of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(22), 3979-3982
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:87056

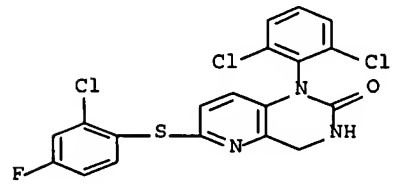
AB Development for a class of potent 3,4-dihydropyrido(3,2-d)pyrimidone inhibitors of p38a MAP kinase is described. Modification of N-1 aryl and C-6 arylsulfide in 3,4-dihydropyrido(3,2-d)pyrimidone analogs for the interaction with the hydrophobic pockets in p38 active site is also discussed.

IT **547756-17-2**
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation and structure-activity relationship of 3,4-dihydropyrido[3,2-d]pyrimidone p38 MAP kinase inhibitors)
RN 547756-17-2 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



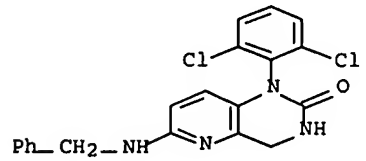
IT **643762-65-6P 643762-85-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and structure-activity relationship of 3,4-dihydropyrido[3,2-d]pyrimidone p38 MAP kinase inhibitors)
RN 643762-65-6 HCAPLUS

CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-chloro-4-fluorophenyl)thio]-1-(2,6-dichlorophenyl)-3,4-dihydro- (9CI) (CA INDEX NAME)



RN 643762-85-0 HCAPLUS

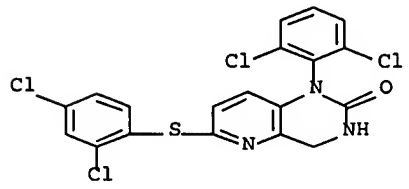
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-3,4-dihydro-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



IT 643762-66-7 643762-67-8 643762-68-9
643762-69-0 643762-70-3 643762-71-4
643762-72-5 643762-73-6 643762-74-7
643762-75-8 643762-76-9 643762-77-0
643762-78-1 643762-79-2 643762-80-5
643762-81-6 643762-82-7 643762-86-1
643762-87-2 643762-88-3 643762-89-4
643762-90-7 643762-91-8 643762-92-9
643762-93-0 643762-94-1 643762-95-2
643762-96-3 643762-97-4 643762-98-5
643762-99-6 643763-00-2 643763-01-3
643763-02-4 643763-03-5 643763-04-6
643763-05-7 643763-07-9 643763-09-1
643763-11-5 643763-13-7 643763-15-9
643763-17-1 643763-19-3 643763-22-8
643763-24-0 643763-26-2 643763-28-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation and structure-activity relationship of 3,4-dihydropyrido[3,2-d]pyrimidone p38 MAP kinase inhibitors)

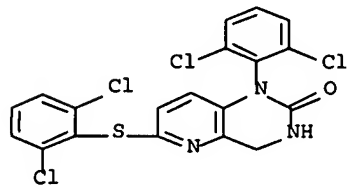
RN 643762-66-7 HCAPLUS

CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-dichlorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



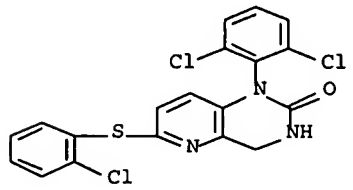
RN 643762-67-8 HCAPLUS

CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,6-dichlorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



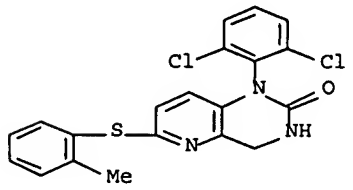
RN 643762-68-9 HCAPLUS

CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-chlorophenyl)thio]-1-(2,6-dichlorophenyl)-3,4-dihydro- (9CI) (CA INDEX NAME)



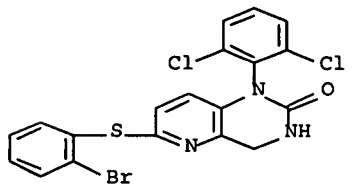
RN 643762-69-0 HCAPLUS

CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-3,4-dihydro-6-[(2-methylphenyl)thio]- (9CI) (CA INDEX NAME)



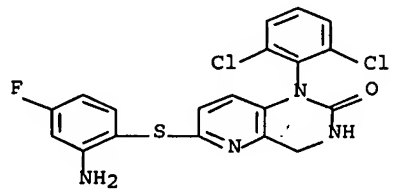
RN 643762-70-3 HCAPLUS

CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-bromophenyl)thio]-1-(2,6-dichlorophenyl)-3,4-dihydro- (9CI) (CA INDEX NAME)

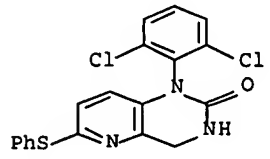


RN 643762-71-4 HCAPLUS

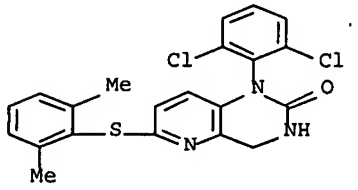
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-amino-4-fluorophenyl)thio]-1-(2,6-dichlorophenyl)-3,4-dihydro- (9CI) (CA INDEX NAME)



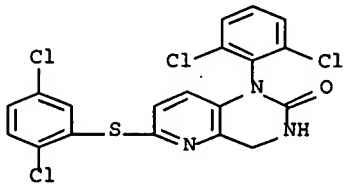
RN 643762-72-5 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-3,4-dihydro-6-(phenylthio)- (9CI) (CA INDEX NAME)



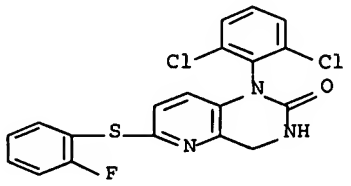
RN 643762-73-6 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,6-dimethylphenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



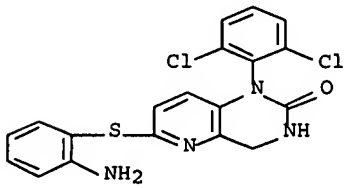
RN 643762-74-7 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,5-dichlorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



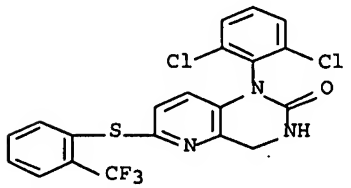
RN 643762-75-8 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2-fluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



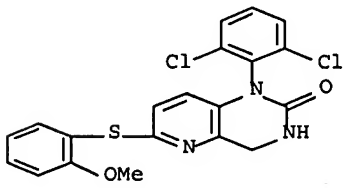
RN 643762-76-9 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-aminophenyl)thio]-1-(2,6-dichlorophenyl)-3,4-dihydro- (9CI) (CA INDEX NAME)



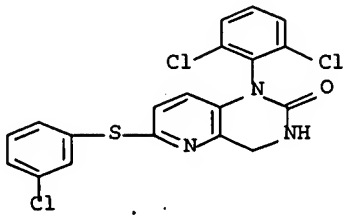
RN 643762-77-0 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-3,4-dihydro-6-[[2-(trifluoromethyl)phenyl]thio]- (9CI) (CA INDEX NAME)



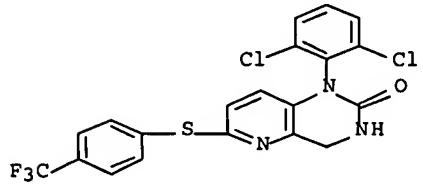
RN 643762-78-1 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-3,4-dihydro-6-[(2-methoxyphenyl)thio]- (9CI) (CA INDEX NAME)



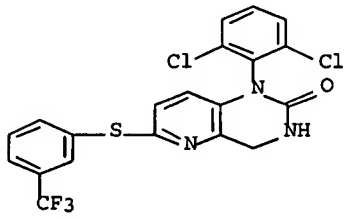
RN 643762-79-2 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(3-chlorophenyl)thio]-1-(2,6-dichlorophenyl)-3,4-dihydro- (9CI) (CA INDEX NAME)



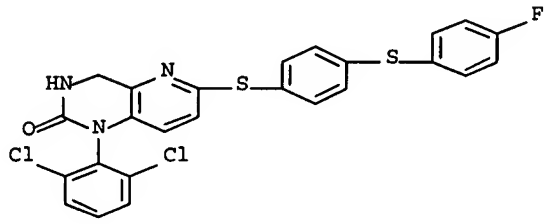
RN 643762-80-5 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-3,4-dihydro-6-[[4-(trifluoromethyl)phenyl]thio]- (9CI) (CA INDEX NAME)



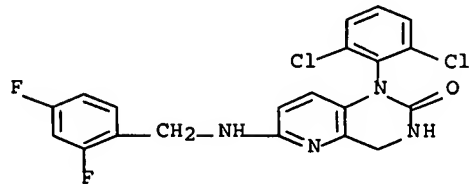
RN 643762-81-6 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-3,4-dihydro-6-[[3-(trifluoromethyl)phenyl]thio]- (9CI) (CA INDEX NAME)



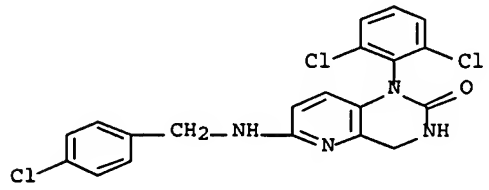
RN 643762-82-7 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[[4-[(4-fluorophenyl)thio]phenyl]thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



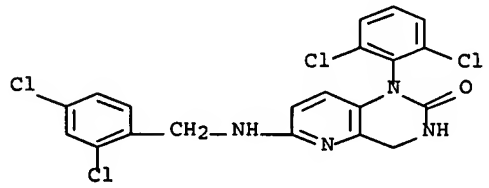
RN 643762-86-1 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[[(2,4-difluorophenyl)methyl]amino]-3,4-dihydro- (9CI) (CA INDEX NAME)



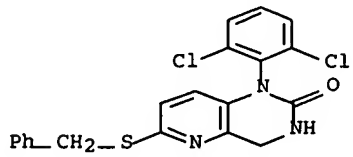
RN 643762-87-2 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[[(4-chlorophenyl)methyl]amino]-1-(2,6-dichlorophenyl)-3,4-dihydro- (9CI) (CA INDEX NAME)



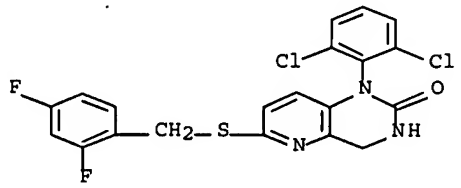
RN 643762-88-3 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[[(2,4-dichlorophenyl)methyl]amino]-3,4-dihydro- (9CI) (CA INDEX NAME)



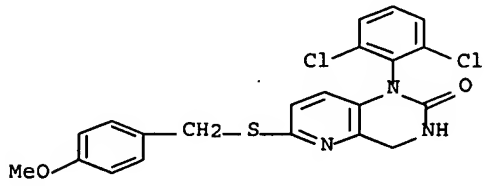
RN 643762-89-4 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-3,4-dihydro-6-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)



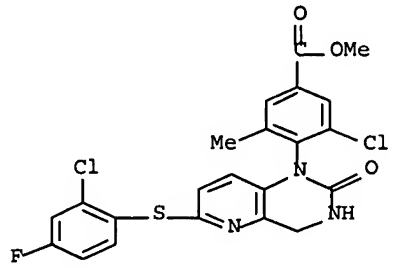
RN 643762-90-7 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[[(2,4-difluorophenyl)methyl]thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



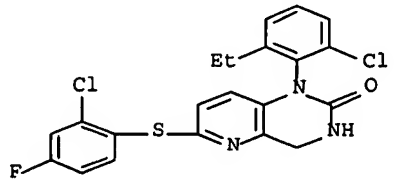
RN 643762-91-8 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-3,4-dihydro-6-[[(4-methoxyphenyl)methyl]thio]- (9CI) (CA INDEX NAME)



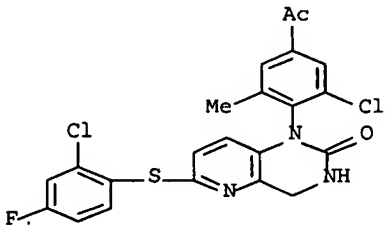
RN 643762-92-9 HCAPLUS
CN Benzoic acid, 3-chloro-4-[6-[(2-chloro-4-fluorophenyl)thio]-3,4-dihydro-2-oxopyrido[3,2-d]pyrimidin-1(2H)-yl]-5-methyl-, methyl ester (9CI) (CA INDEX NAME)



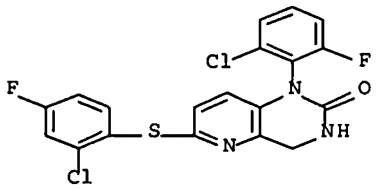
RN 643762-93-0 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2-chloro-6-ethylphenyl)-6-[(2-chloro-4-fluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



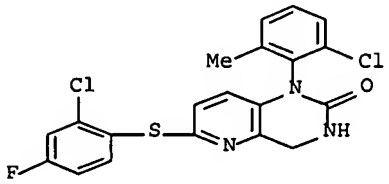
RN 643762-94-1 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(4-acetyl-2-chloro-6-methylphenyl)-6-[(2-chloro-4-fluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



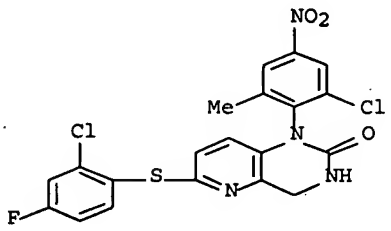
RN 643762-95-2 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2-chloro-6-fluorophenyl)-6-[(2-chloro-4-fluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



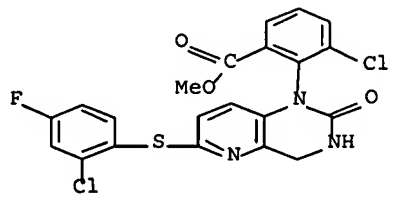
RN 643762-96-3 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-chloro-4-fluorophenyl)thio]-1-(2-chloro-6-methylphenyl)-3,4-dihydro- (9CI) (CA INDEX NAME)



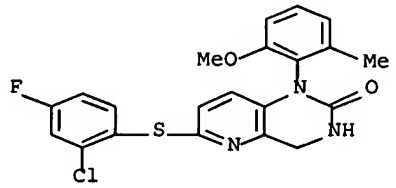
RN 643762-97-4 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-chloro-4-fluorophenyl)thio]-1-(2-chloro-6-methyl-4-nitrophenyl)-3,4-dihydro- (9CI) (CA INDEX NAME)



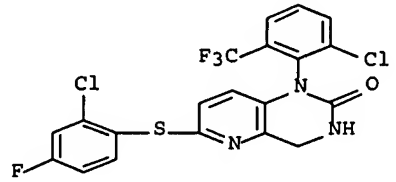
RN 643762-98-5 HCAPLUS
CN Benzoic acid, 3-chloro-2-[6-[(2-chloro-4-fluorophenyl)thio]-3,4-dihydro-2-oxopyrido[3,2-d]pyrimidin-1(2H)-yl]-, methyl ester (9CI) (CA INDEX NAME)



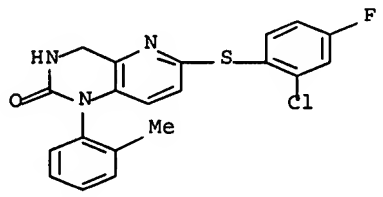
RN 643762-99-6 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-chloro-4-fluorophenyl)thio]-3,4-dihydro-1-(2-methoxy-6-methylphenyl)- (9CI) (CA INDEX NAME)



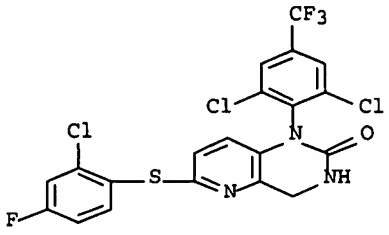
RN 643763-00-2 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-chloro-4-fluorophenyl)thio]-1-[2-chloro-6-(trifluoromethyl)phenyl]-3,4-dihydro- (9CI) (CA INDEX NAME)



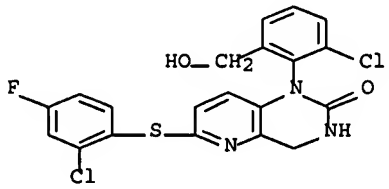
RN 643763-01-3 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-chloro-4-fluorophenyl)thio]-3,4-dihydro-1-(2-methylphenyl)- (9CI) (CA INDEX NAME)



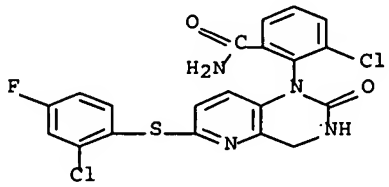
RN 643763-02-4 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-chloro-4-fluorophenyl)thio]-1-[2,6-dichloro-4-(trifluoromethyl)phenyl]-3,4-dihydro- (9CI) (CA INDEX NAME)



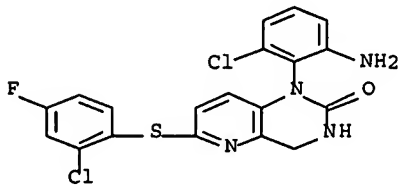
RN 643763-03-5 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-chloro-4-fluorophenyl)thio]-1-[2-chloro-6-(hydroxymethyl)phenyl]-3,4-dihydro- (9CI) (CA INDEX NAME)



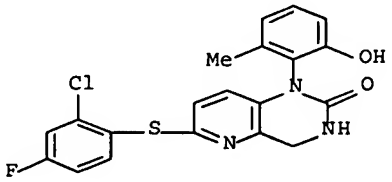
RN 643763-04-6 HCAPLUS
CN Benzamide, 3-chloro-2-[6-[(2-chloro-4-fluorophenyl)thio]-3,4-dihydro-2-oxopyrido[3,2-d]pyrimidin-1(2H)-yl]- (9CI) (CA INDEX NAME)



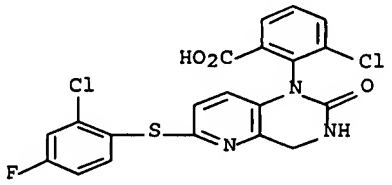
RN 643763-05-7 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2-amino-6-chlorophenyl)-6-[(2-chloro-4-fluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



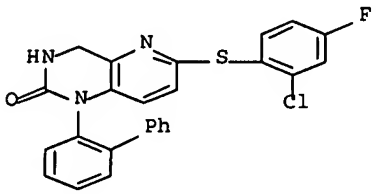
RN 643763-07-9 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-chloro-4-fluorophenyl)thio]-3,4-dihydro-1-(2-hydroxy-6-methylphenyl)- (9CI) (CA INDEX NAME)



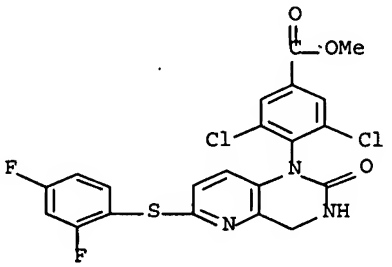
RN 643763-09-1 HCAPLUS
CN Benzoic acid, 3-chloro-2-[6-[(2-chloro-4-fluorophenyl)thio]-3,4-dihydro-2-oxopyrido[3,2-d]pyrimidin-1(2H)-yl]- (9CI) (CA INDEX NAME)



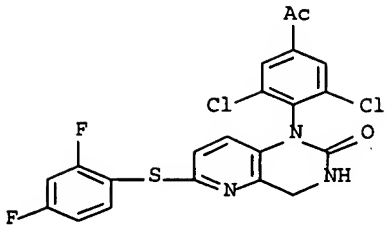
RN 643763-11-5 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-[1,1'-biphenyl]-2-yl-6-[(2-chloro-4-fluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



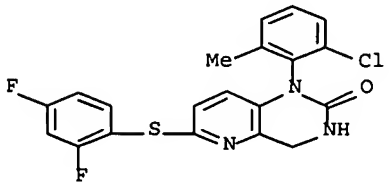
RN 643763-13-7 HCAPLUS
CN Benzoic acid, 3,5-dichloro-4-[6-[(2,4-difluorophenyl)thio]-3,4-dihydro-2-oxopyrido[3,2-d]pyrimidin-1(2H)-yl]-, methyl ester (9CI) (CA INDEX NAME)



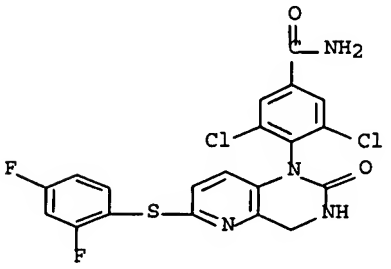
RN 643763-15-9 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(4-acetyl-2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



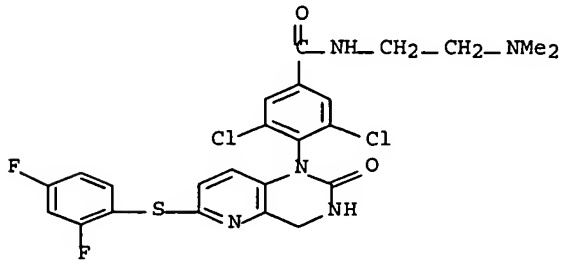
RN 643763-17-1 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2-chloro-6-methylphenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



RN 643763-19-3 HCAPLUS
CN Benzamide, 3,5-dichloro-4-[6-[(2,4-difluorophenyl)thio]-3,4-dihydro-2-oxopyrido[3,2-d]pyrimidin-1(2H)-yl]- (9CI) (CA INDEX NAME)

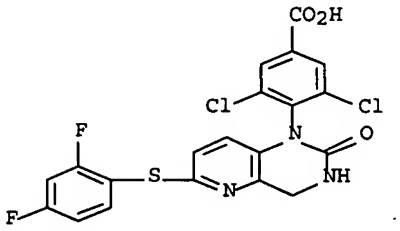


RN 643763-22-8 HCAPLUS
CN Benzamide, 3,5-dichloro-4-[6-[(2,4-difluorophenyl)thio]-3,4-dihydro-2-oxopyrido[3,2-d]pyrimidin-1(2H)-yl]-N-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

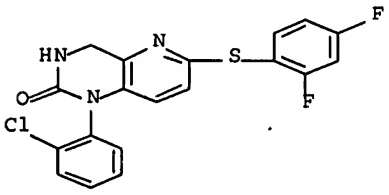


RN 643763-24-0 HCAPLUS

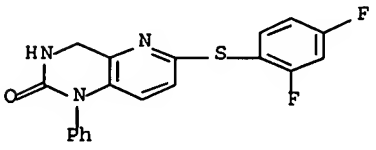
CN Benzoic acid, 3,5-dichloro-4-[6-[(2,4-difluorophenyl)thio]-3,4-dihydro-2-oxopyrido[3,2-d]pyrimidin-1(2H)-yl]- (9CI) (CA INDEX NAME)



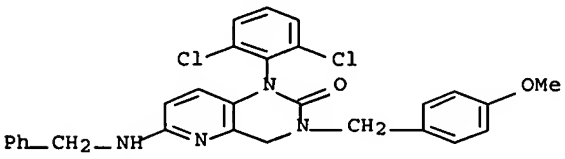
RN 643763-26-2 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2-chlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



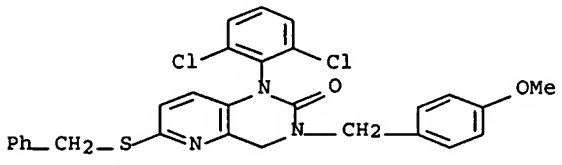
RN 643763-28-4 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2,4-difluorophenyl)thio]-3,4-dihydro-1-phenyl- (9CI) (CA INDEX NAME)



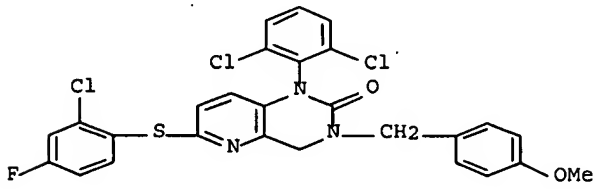
IT **720665-80-5 720665-83-8 720665-79-2P**
RL: RCT (Reactant); SPN (Synthetic preparation)
(preparation and structure-activity relationship of 3,4-dihydropyrido[3,2-d]pyrimidone p38 MAP kinase inhibitors)
RN 720665-80-5 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-3,4-dihydro-3-[(4-methoxyphenyl)methyl]-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 720665-83-8 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-3,4-dihydro-3-[(4-methoxyphenyl)methyl]-6-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)



RN 720665-79-2 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 6-[(2-chloro-4-fluorophenyl)thio]-1-(2,6-dichlorophenyl)-3,4-dihydro-3-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



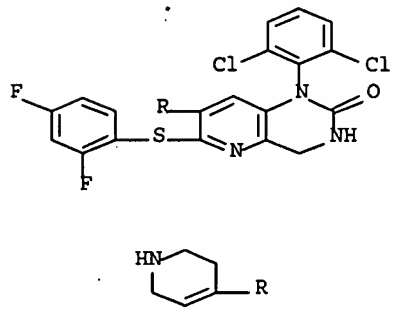
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 13 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:665748 HCAPLUS Full-text
DOCUMENT NUMBER: 139:334683
TITLE: Structural basis for p38α MAP kinase quinazolinone and pyridol-pyrimidine inhibitor specificity
AUTHOR(S): Fitzgerald, Catherine E.; Patel, Sangita B.; Becker, Joseph W.; Cameron, Patricia M.; Zaller, Dennis; Pikounis, Vasilis Bill; O'Keefe, Stephen J.; Scapin, Giovanna
CORPORATE SOURCE: Departments of Immunology and Rheumatology, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Nature Structural Biology (2003), 10(9), 764-769
CODEN: NSBIEW; ISSN: 1072-8368
PUBLISHER: Nature Publishing Group
DOCUMENT TYPE: Journal
LANGUAGE: English

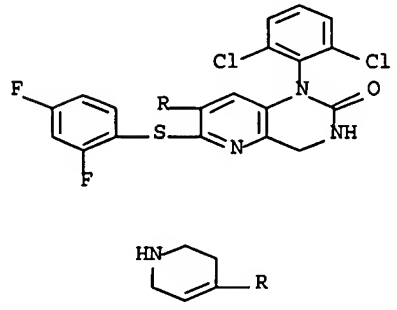
AB The quinazolinone and pyridol-pyrimidine classes of p38 MAP kinase inhibitors have a previously unseen degree of specificity for p38 over other MAP kinases. Comparison of the crystal structures of p38 bound to four different compds. shows that binding of the more specific mols. is characterized by a peptide flip between Met109 and Gly110. Gly110 is a residue specific to the α, β and γ isoforms of p38. The δ isoform and the other MAP kinases have bulkier residues in this position. These residues would likely make the peptide flip energetically unfavorable, thus explaining the selectivity of binding. To test this hypothesis, we constructed G110A and G110D mutants of p38 and measured the potency of several compds. against them. The results confirm that the selectivity of quinazolinones and pyridol-pyrimidines results from the presence of a glycine in position 110. This unique mode of binding may be exploited in the design of new p38 inhibitors.

IT 616894-42-9 616894-42-9D, complexes with p38α MAP kinase
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(Gly110 residue of p38α MAP kinase plays role in selectivity of quinazolinone and pyridol-pyrimidine inhibitors through hydrogen bonding)

RN 616894-42-9 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-(1,2,3,6-tetrahydro-4-pyridinyl)-(9CI) (CA INDEX NAME)



RN 616894-42-9 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-(1,2,3,6-tetrahydro-4-pyridinyl)-(9CI) (CA INDEX NAME)



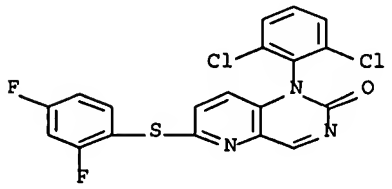
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 14 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:943601 HCAPLUS Full-text
DOCUMENT NUMBER: 139:46382
TITLE: p38 MAP kinase inhibitors. Part 1: design and development of a new class of potent and highly selective inhibitors based on 3,4-dihydropyrido[3,2-d]pyrimidone scaffold
AUTHOR(S): Natarajan, Swaminathan R.; Wisnoski, David D.; Singh, Suresh B.; Stelmach, John E.; O'Neill, Edward A.; Schwartz, Cheryl D.; Thompson, Chris M.; Fitzgerald, Catherine E.; O'Keefe, Stephen J.; Kumar, Sanjeev; Hop, Cornelis E. C. A.; Zaller, Dennis M.; Schmatz, Dennis M.; Doherty,

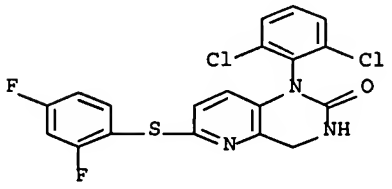
James B.
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(2), 273-276
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:46382

AB A new class of p38 antagonists based on 3,4-dihydropyrido[3,2,- d]pyrimidine scaffold has been developed. These inhibitors exhibit unprecedented selectivity towards p38 over other very closely related kinases. Three compds. were identified as benchmark analogs for follow-up studies. They show good potency for enzyme inhibition and excellent functional activity.

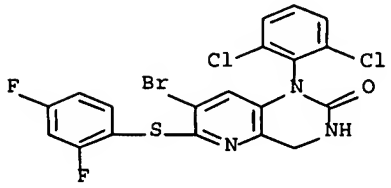
IT **547756-18-3**
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(p38 MAP kinase inhibitors: design of potent and selective inhibitors based on 3,4-dihydropyrido[3,2-d]pyrimidone scaffold)
RN 547756-18-3 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]- (9CI) (CA INDEX NAME)



IT **547756-17-2P 547756-25-2P**
RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(p38 MAP kinase inhibitors: design of potent and selective inhibitors based on 3,4-dihydropyrido[3,2-d]pyrimidone scaffold)
RN 547756-17-2 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



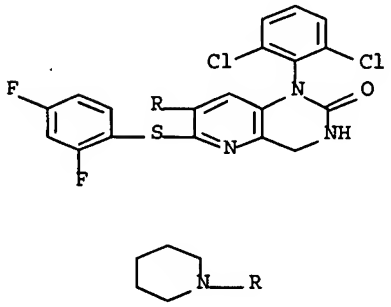
RN 547756-25-2 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 7-bromo-1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



IT 547756-26-3P 547756-27-4P 547756-28-5P
547756-29-6P 547756-30-9P 547756-31-0P
547756-32-1P 547756-33-2P 547756-34-3P
547756-35-4P 547756-36-5P 547756-37-6P
547756-39-8P 547756-40-1P 547756-41-2P
547756-42-3P 547756-43-4P 547756-44-5P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(p38 MAP kinase inhibitors: design of potent and selective inhibitors based on 3,4-dihydropyrido[3,2-d]pyrimidone scaffold)

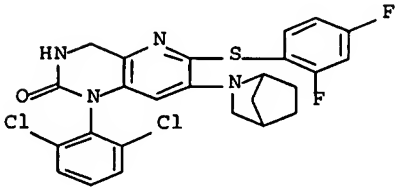
RN 547756-26-3 HCAPLUS

CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-(1-piperidinyl)- (9CI) (CA INDEX NAME)



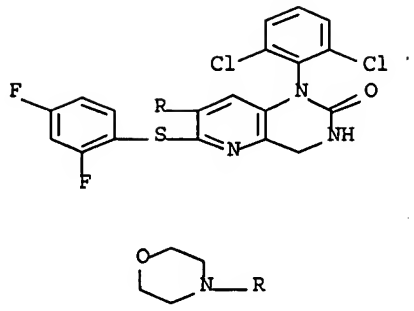
RN 547756-27-4 HCAPLUS

CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 7-(2-azabicyclo[2.2.1]hept-2-yl)-1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)

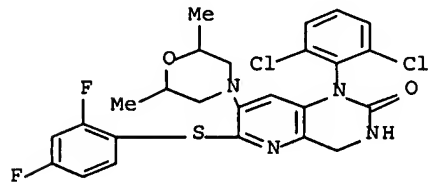


RN 547756-28-5 HCAPLUS

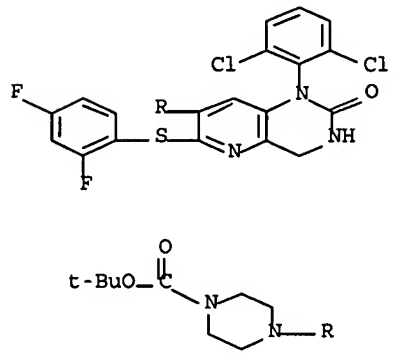
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-(4-morpholinyl)- (9CI) (CA INDEX NAME)



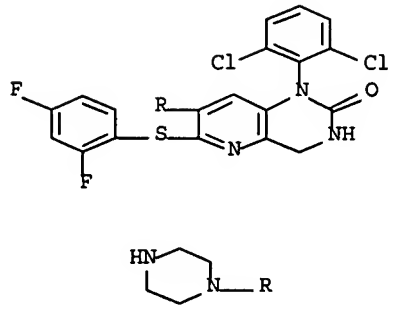
RN 547756-29-6 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-7-(2,6-dimethyl-4-morpholinyl)-3,4-dihydro- (9CI) (CA INDEX NAME)



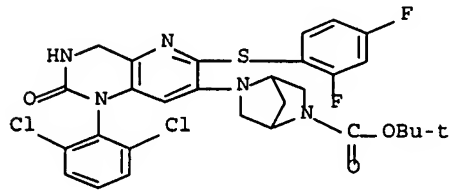
RN 547756-30-9 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-1,2,3,4-tetrahydro-2-oxopyrido[3,2-d]pyrimidin-7-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



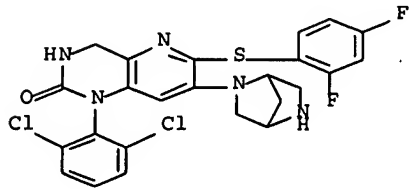
RN 547756-31-0 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-(1-piperazinyl)- (9CI) (CA INDEX NAME)



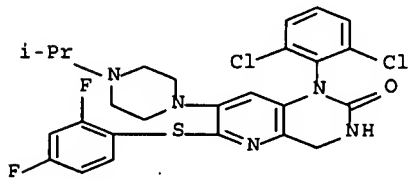
RN 547756-32-1 HCAPLUS
CN 2,5-Diazabicyclo[2.2.1]heptane-2-carboxylic acid, 5-[1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-1,2,3,4-tetrahydro-2-oxopyrido[3,2-d]pyrimidin-7-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



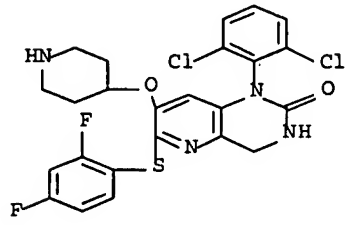
RN 547756-33-2 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 7-(2,5-diazabicyclo[2.2.1]hept-2-yl)-1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



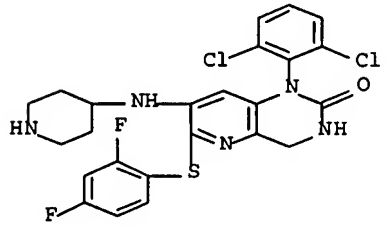
RN 547756-34-3 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-[4-(1-methylethyl)-1-piperazinyl]- (9CI) (CA INDEX NAME)



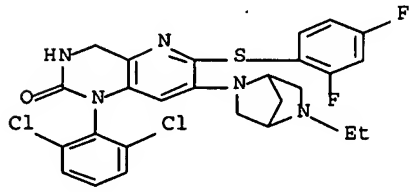
RN 547756-35-4 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-(4-piperidinyloxy)- (9CI) (CA INDEX NAME)



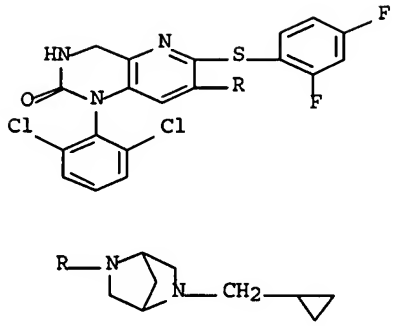
RN 547756-36-5 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-(4-piperidinylamino)- (9CI) (CA INDEX NAME)



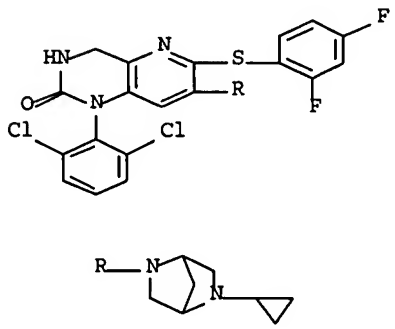
RN 547756-37-6 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-7-(5-ethyl-2,5-diazabicyclo[2.2.1]hept-2-yl)-3,4-dihydro- (9CI) (CA INDEX NAME)



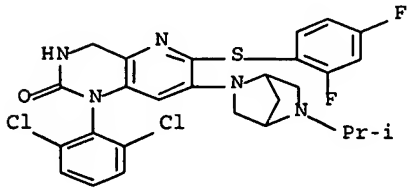
RN 547756-39-8 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 7-[5-(cyclopropylmethyl)-2,5-diazabicyclo[2.2.1]hept-2-yl]-1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



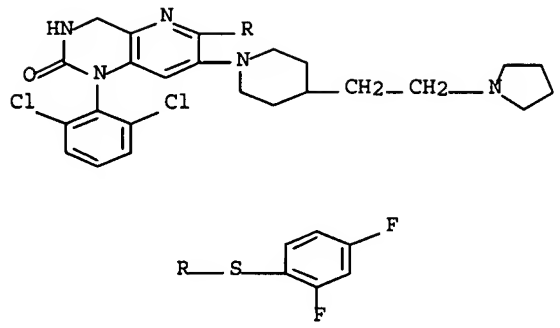
RN 547756-40-1 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 7-(5-cyclopropyl-2,5-diazabicyclo[2.2.1]hept-2-yl)-1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



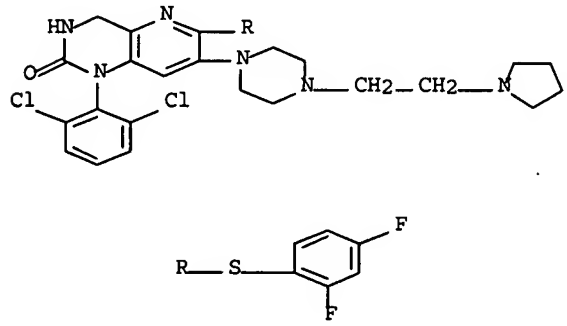
RN 547756-41-2 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-[5-(1-methylethyl)-2,5-diazabicyclo[2.2.1]hept-2-yl]- (9CI) (CA INDEX NAME)



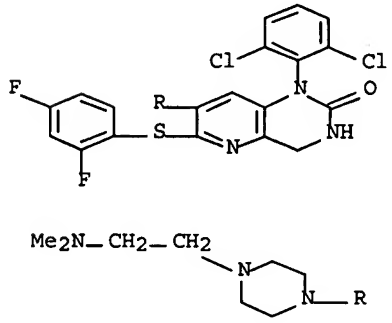
RN 547756-42-3 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-[4-[2-(1-pyrrolidinyl)ethyl]-1-piperidinyl]- (9CI) (CA INDEX NAME)



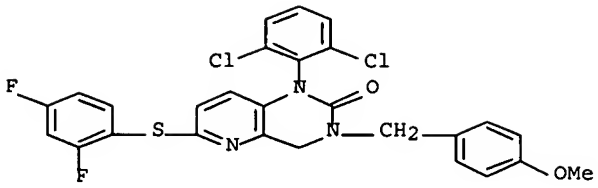
RN 547756-43-4 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-7-[4-[2-(1-pyrrolidinyl)ethyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)



RN 547756-44-5 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-7-[4-[2-(dimethylamino)ethyl]-1-piperazinyl]-3,4-dihydro- (9CI) (CA INDEX NAME)



IT **547756-24-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(p38 MAP kinase inhibitors: design of potent and selective inhibitors based on 3,4-dihydropyrido[3,2-d]pyrimidone scaffold)
RN 547756-24-1 HCAPLUS
CN Pyrido[3,2-d]pyrimidin-2(1H)-one, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro-3-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



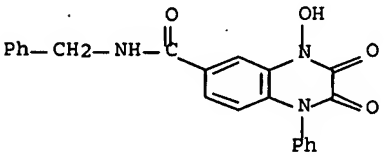
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 15 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:338061 HCAPLUS Full-text
DOCUMENT NUMBER: 137:310892
TITLE: Solid-phase synthesis of 'diverse' heterocycles
AUTHOR(S): Purandare, Ashok V.; Gao, Aiming; Poss, Michael A.
CORPORATE SOURCE: New Leads Chemistry, Bristol-Myers Squibb PRI, Princeton, NJ, 08543, USA
SOURCE: Tetrahedron Letters (2002), 43(21), 3903-3906
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:310892

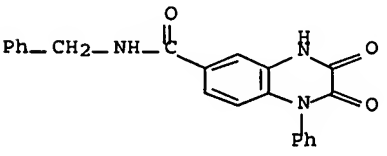
AB Diverse heterocycles, i.e., quinoxalinediones, quinoxalinones, benzimidazolones, and benzimidazoles, were prepared from 4-fluoro-3-nitrobenzoic acid by solid-phase synthesis on polymer-supported aminomethylphenol.

IT **471891-57-3P 471891-60-8P 471891-61-9P 471891-62-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase synthesis of quinoxalinediones, quinoxalinones, benzimidazolones, and benzimidazoles)

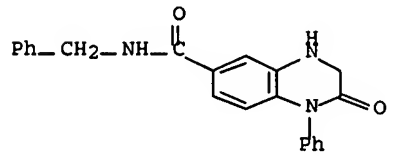
RN 471891-57-3 HCAPLUS
CN 6-Quinoxalinecarboxamide, 1,2,3,4-tetrahydro-4-hydroxy-2,3-dioxo-1-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



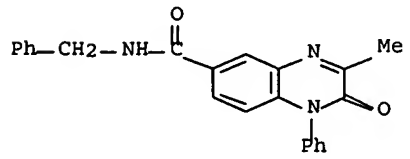
RN 471891-60-8 HCAPLUS
CN 6-Quinoxalinecarboxamide, 1,2,3,4-tetrahydro-2,3-dioxo-1-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 471891-61-9 HCAPLUS
CN 6-Quinoxalinecarboxamide, 1,2,3,4-tetrahydro-2-oxo-1-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 471891-62-0 HCAPLUS
CN 6-Quinoxalinecarboxamide, 1,2-dihydro-3-methyl-2-oxo-1-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 16 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:396853 HCAPLUS Full-text
DOCUMENT NUMBER: 135:19654
TITLE: 3,4-Dihydro-(1H)-quinazolin-2-ones and their use as CSBP/p38 kinase inhibitors
INVENTOR(S): Adams, Jerry L.; Bower, Michael J.; Boehm, Jeffrey Charles; Griswold, Don E.; Underwood, David C.
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

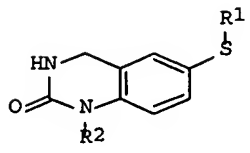
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001038314	A1	20010531	WO 2000-US31894	200011 21

W: AE, AL, AU, BA, BB, BG, BR, BZ, CA, CN, CZ, DZ, EE, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, MZ, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, TZ, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

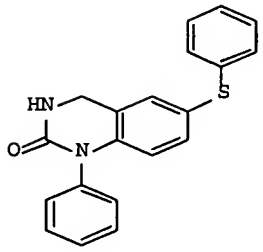
AU 200117832	A	20010604	AU 2001-17832	200011 21
EP 1233951	A1	20020828	EP 2000-980587	200011 21
EP 1233951	B1	20050601		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003514900	T	20030422	JP 2001-540077	200011 21
AT 296809	T	20050615	AT 2000-980587	200011 21
ES 2241675	T3	20051101	ES 2000-980587	200011 21
US 7053098	B1	20060530	US 2002-129888	200205 10
PRIORITY APPLN. INFO.:			US 1999-166975P P	199911 23
			WO 2000-US31894 W	200011 21

OTHER SOURCE(S): MARPAT 135:19654

GI



I



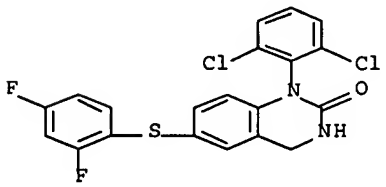
II

AB Novel substituted quinazoline compds. are disclosed, specifically I [R1 = (un)substituted Ph, naphthyl, heterocyclyl or heteroaryl; R2 = (un)substituted alkyl, (hetero)aryl(alkyl), or heterocyclyl(alkyl)] and their pharmaceutically acceptable salts. Also disclosed are pharmaceutical compns. containing I, and use of I in therapy as CSBP/RK/p38 kinase inhibitors. Applications of I as such to a wide variety of arthritic, inflammatory, proliferative, and viral conditions are specifically claimed. Also claimed is use of I in conjunction with various other drugs or drug classes, and a process for preparation of I from corresponding 2-amino-5-(substituted-thio)benzonitriles via reduction and cyclization. Three examples of I were prepared and specifically claimed. For instance, 2-chloro-5-nitrobenzonitrile was condensed with aniline at Cl, followed by reduction of the nitro group to amino, diazotization of amino, coupling of the diazonium salt with thiophenol, reduction of the nitrile to aminomethyl using LiAlH4, and cyclocondensation of the resultant diamine with carbonyldiimidazole, to give title compound II. Representative compds. I had IC50 values < 50 μM in a CSBP/p38 kinase assay.

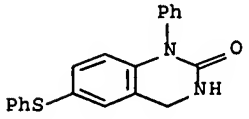
IT **252265-88-6P 342433-95-8P 342433-96-9P**
RL: BAC (Biological activity or effector, except adverse); BSU

(Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of dihydroquinazolinones as CSBP/RK/p38 kinase inhibitors)

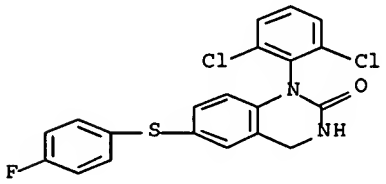
RN 252265-88-6 HCAPLUS
CN 2(1H)-Quinazolinone, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



RN 342433-95-8 HCAPLUS
CN 2(1H)-Quinazolinone, 3,4-dihydro-1-phenyl-6-(phenylthio)- (9CI) (CA INDEX NAME)



RN 342433-96-9 HCAPLUS
CN 2(1H)-Quinazolinone, 1-(2,6-dichlorophenyl)-6-[(4-fluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



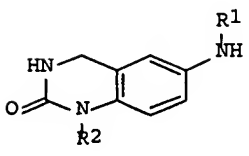
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 17 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:396852 HCAPLUS Full-text
DOCUMENT NUMBER: 135:19653
TITLE: 3,4-Dihydro-(1H)-quinazolin-2-ones and their use as CSBP/p38 kinase inhibitors
INVENTOR(S): Adams, Jerry L.; Bower, Michael J.; Boehm, Jeffrey Charles; Griswold, Don E.; Underwood, David C.
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, UK
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

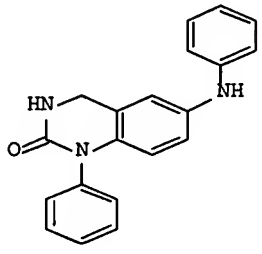
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001038313	A1	20010531	WO 2000-US31874	200011 21
W: AE, AL, AU, BA, BB, BG, BR, BZ, CA, CN, CZ, DZ, EE, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, MZ, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, TZ, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1233950	A1	20020828	EP 2000-980576	200011 21
EP 1233950	B1	20051005		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003528043	T	20030924	JP 2001-540076	200011 21
AT 305787	T	20051015	AT 2000-980576	200011 21
ES 2249309	T3	20060401	ES 2000-980576	200011 21
US 6982270	B1	20060103	US 2002-129863	200205 10
PRIORITY APPLN. INFO.:			US 1999-166972P P	199911 23
			WO 2000-US31874 W	200011 21

OTHER SOURCE(S): MARPAT 135:19653
GI



I



II

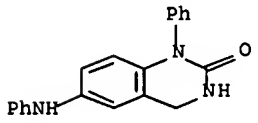
AB Novel substituted quinazoline compds. are disclosed, specifically I [R1 = (un)substituted Ph, naphthyl, heterocyclyl or heteroaryl; R2 = (un)substituted alkyl, (hetero)aryl(alkyl), or heterocyclyl(alkyl)] and their pharmaceutically acceptable

salts. Also disclosed are pharmaceutical compns. containing I, and use of I in therapy as CSBP/RK/p38 kinase inhibitors. Applications of I as such to a wide variety of arthritic, inflammatory, proliferative, and viral conditions are specifically claimed. Also claimed is use of I in conjunction with various other drugs or drug classes, and a process for preparing I by cyclization of corresponding diaminobenzylamine derivs. with carbonyldiimidazole or its analogs. A single example of I was prepared and claimed. Thus, 2-chloro-5-nitrobenzonitrile underwent a sequence of: (1) condensation with aniline at Cl; (2) reduction of nitro to amino; (3) arylation of amino with PhB(OH)2 and Cu(OAc)2; (4) hydrogenation of the nitrile to aminomethyl; and (5) cyclocondensation with carbonyldiimidazole, to give title compound II. Representative compds. I had IC50 values < 50 μM in a CSBP/p38 kinase assay.

IT **342433-64-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of dihydroquinazolinones as CSBP/RK/p38 kinase inhibitors)

RN 342433-64-1 HCAPLUS

CN 2(1H)-Quinazolinone, 3,4-dihydro-1-phenyl-6-(phenylamino)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 18 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:795793 HCAPLUS Full-text
DOCUMENT NUMBER: 132:30857
TITLE: Heterocyclic compound inhibitors of p38 kinase, pharmaceutical compositions, and therapeutic use
INVENTOR(S): Salituro, Francesco; Bemis, Guy; Cochran, John
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 68 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9964400	A1	19991216	WO 1999-US12951	19990611
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9944297	A	19991230	AU 1999-44297	19990611
EP 1086085	A1	20010328	EP 1999-927377	

					199906 11
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI					
EP 1277740		A1	20030122	EP 2002-22891	
					199906 11
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY					
US 2001025044		A1	20010927	US 2000-734069	
					200012 11
US 6528508		B2	20030304		
US 2003149037		A1	20030807	US 2002-327020	
					200212 20
US 6800626		B2	20041005		
US 2005049251		A1	20050303	US 2004-951409	
					200409 27
US 7151101		B2	20061219		
PRIORITY APPLN. INFO.:				US 1998-89147P	P
					199806 12
				EP 1999-927377	A3
					199906 11
				WO 1999-US12951	W
					199906 11
				US 2000-734069	A3
					200012 11
				US 2002-327020	A3
					200212 20

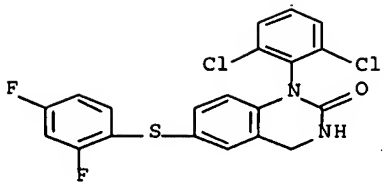
OTHER SOURCE(S): MARPAT 132:30857

AB The invention relates to heterocyclic compound inhibitors of p38, a mammalian protein kinase involved cell proliferation, cell death and response to extracellular stimuli. The invention also relates to methods for producing these inhibitors. The invention also provides pharmaceutical compns. comprising the inhibitors of the invention and methods of utilizing those compns. in the treatment and prevention of various disorders.

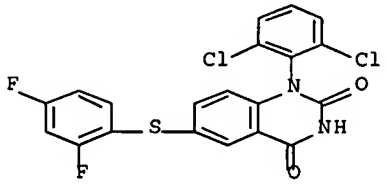
IT **252265-88-6 252265-89-7**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(heterocyclic compound inhibitors of p38 kinase, pharmaceutical compns., and therapeutic use)

RN 252265-88-6 HCAPLUS

CN 2(1H)-Quinazolinone, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]-3,4-dihydro- (9CI) (CA INDEX NAME)



RN 252265-89-7 HCAPLUS
CN 2,4(1H,3H)-Quinazolinedione, 1-(2,6-dichlorophenyl)-6-[(2,4-difluorophenyl)thio]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 19 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:421302 HCAPLUS Full-text
DOCUMENT NUMBER: 127:34143
TITLE: Farnesyl transferase inhibiting 2-quinolone derivatives
INVENTOR(S): End, David William; Venet, Marc Gaston; Angibaud, Patrick Rene; Sanz, Gerard Charles
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

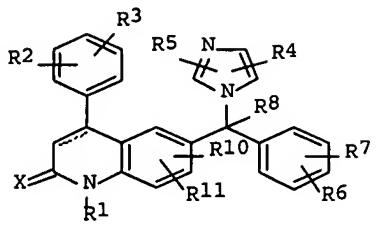
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9716443	A1	19970509	WO 1996-EP4661	19961025
W: AL, AM, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KG, KR, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AZ, BY, KZ, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2231143	C	19970509	CA 1996-2231143	19961025
CA 2231143	A1	19970509		
AU 9674933	A	19970522	AU 1996-74933	19961025
AU 712435	B2	19991104		

CN 1200732	A	19981202	CN 1996-197917	199610 25
CN 1101391	B	20030212		
HU 9802424	A2	19991028	HU 1998-2424	199610 25
HU 224032	B1	20050530		
JP 11514635	T	19991214	JP 1997-517051	199610 25
EP 1019395	A1	20000719	EP 1996-937249	199610 25
EP 1019395	B1	20020130		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
EP 1106610	A1	20010613	EP 2001-200450	199610 25
EP 1106610	B1	20040616		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
AT 212627	T	20020215	AT 1996-937249	199610 25
PT 1019395	T	20020731	PT 1996-937249	199610 25
ES 2171736	T3	20020916	ES 1996-937249	199610 25
PL 184168	B1	20020930	PL 1996-328230	199610 25
SK 282642	B6	20021008	SK 1998-556	199610 25
IL 123567	A	20021110	IL 1996-123567	199610 25
CZ 290954	B6	20021113	CZ 1998-1272	199610 25
AT 269322	T	20040715	AT 2001-200450	199610 25
ES 2233557	T3	20050616	ES 2001-200450	199610 25
ZA 9609087	A	19980429	ZA 1996-9087	199610 29
IN 1996CA01881	A	20050304	IN 1996-CA1881	199610 31
NO 9800928	A	19980429	NO 1998-928	199803 04
NO 314037	B1	20030120		
US 5968952	A	19991019	US 1998-66441	199804 29
HK 1027576	A1	20020524	HK 2000-106863	200010 27
HK 1036064	A1	20041119	HK 2001-106814	

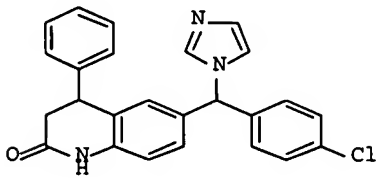
PRIORITY APPLN. INFO.: EP 1995-202945 A 200109 27
EP 1996-937249 A3 199510 31
WO 1996-EP4661 W 199610 25
199610 25

OTHER SOURCE(S): MARPAT 127:34143

GI



I



II

AB The invention concerns compds. I and their stereoisomers and pharmaceutically acceptable acid or base addition salts [wherein dotted line = optional pi bond; X = O, S; R1-R11 = H, variety of substituents; adjacent R2R3 may form a bivalent radical]. I are inhibitors of farnesyl protein transferase (FPT), and are thus useful as inhibitors of tumors, other malignant and benign proliferative diseases, and angiogenesis. For instance, 3,4-dihydro-4-phenyl-2(1H)-quinolinone was acylated by 4-ClC6H4CO2H and polyphosphoric acid. The resulting ketone was reduced to an alc. with NaBH4, and the alc. was treated with NaH and 1,1'-carbonylbis-1H-imidazole to give title compound II. Selected I had IC50 values of 0.0034-3.2 μM for inhibition of FPT in vitro. In a ras-transformed cell phenotype reversion assay, selected I had IC50 values as low as 53 nM.

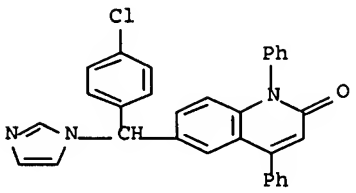
IT **190897-67-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinolone derivs. as farnesyl transferase inhibitors)

RN 190897-67-7 HCAPLUS

CN 2(1H)-Quinolinone, 6-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-1,4-diphenyl-, mononitrate (9CI) (CA INDEX NAME)

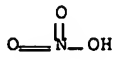
CM 1

CRN 190897-66-6
CMF C31 H22 Cl N3 O



CM 2

CRN 7697-37-2
CMF H N O3

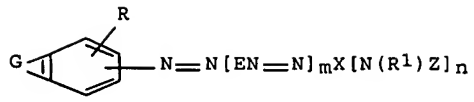


L10 ANSWER 20 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:994572 HCAPLUS Full-text
DOCUMENT NUMBER: 124:31992
TITLE: Water-soluble azo compounds, their preparation and their use as reactive dyes.
INVENTOR(S): Schumacher, Christian; Russ, Werner Hubert
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Eur. Pat. Appl., 39 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 675172	A2	19951004	EP 1995-100784	19950120
EP 675172	A3	19980325		
EP 675172	B1	20010411		
R: BE, CH, DE, FR, GB, LI, NL				
DE 4403395	A1	19950810	DE 1994-4403395	19940204
DE 4442947	A1	19960605	DE 1994-4442947	19941202

PRIORITY APPLN. INFO.: DE 1994-4403395 A 19940204
DE 1994-4442947 A 19941202

OTHER SOURCE(S): MARPAT 124:31992
GI



I

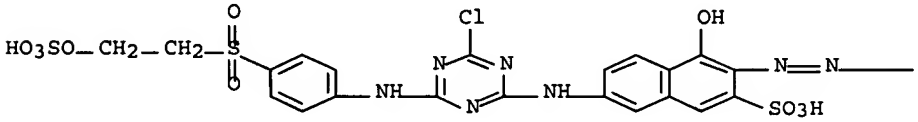
AB The dyes (I; E = aniline- or naphthylamine-based connecting group; G = saturated heterocycle-forming linkage containing N, CO, and other group; R = H, alkyl, alkoxy, halo, sulfo; R1 = H, organic group; X = aniline- or naphthylamine- or heterocycle-based connecting group; Z = fiber-reactive group; m = 0-2; n = 1-4) are obtained by diazotization and coupling and use of fiber-reactive compds. I are used to give fast dyeings and prints on cellulosics. Thus, cyanuric chloride was condensed with aniline-2,5-disulfonic acid and 3-amino-8-hydroxy-6-sulfonaphthalene and the product was coupled with diazotized 5-amino-2-benzimidazolone to give a dye (λmax 516 nm).

IT **171727-79-0P**
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(preparation of water-soluble reactive azo dyes for cellulosics)

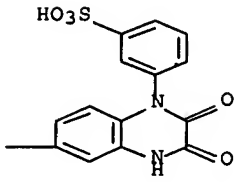
RN 171727-79-0 HCAPLUS

CN 2-Naphthalenesulfonic acid, 7-[[4-chloro-6-[[4-[[2-(sulfooxy)ethyl]sulfonyl]phenyl]amino]-1,3,5-triazin-2-yl]amino]-4-hydroxy-3-[[1,2,3,4-tetrahydro-2,3-dioxo-1-(3-sulfophenyl)-6-quinoxalinyl]azo]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

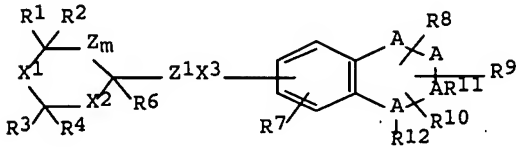


L10 ANSWER 21 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:789143 HCAPLUS Full-text
DOCUMENT NUMBER: 123:198641
TITLE: Preparation of heteroarylquinolines as leukotriene biosynthesis inhibitors
INVENTOR(S): Friesen, Rick; Young, Robert N.; Girard, Yves; Blouin, Marc; Dube, Daniel
PATENT ASSIGNEE(S): Merck Frosst Canada Inc., Can.
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

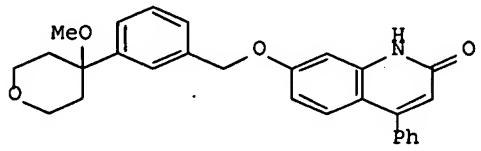
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9503300	A1	19950202	WO 1994-CA388	199407 15
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, FI, GE, HU, JP, KE, KG, KR, KZ, LK, LT, LV, MD, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SI, SK, TJ, TT, UA, US, UZ				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5410054	A	19950425	US 1993-95131	199307 20
CA 2167317	A1	19950202	CA 1994-2167317	199407 15
AU 9472612	A	19950220	AU 1994-72612	199407 15
PRIORITY APPLN. INFO.:			US 1993-95131 A	199307 20
			WO 1994-CA388 W	199407 15

OTHER SOURCE(S): MARPAT 123:198641

GI



I



II

AB Title compds. [I; 1 of A = N and the others = C; Z = CHR5; R1,R5 = H, OH, alkyl, alkoxy; R2,R4 = H, alkyl; R1R2 = O; R3 = H, (hydroxy)alkyl, alkoxyalkyl; R1R3 = (oxy)alk(en)ylene; R6 = H, OH, alkyl, alkoxy, alkylthio, alkanoyloxy; R7 = H, halo, alkyl, OH, alkoxy, etc.; R8 = H, halo, CF3, alkoxy, etc.; R9,R10 = H, alkyl, heteroaryl, etc.; R11,R12 = H; R11R12 = bond; X1 = O, SO0-2, CH2; X2 = O, S, CH2, (cyclo)alkylidene; X3 = (cyclo)alkylideneoxy, -thio, etc.; Z1 = arylene; m = 0 or 1] were prepared as leukotriene biosynthesis inhibitors (no data). Thus, PhCOCH2CO2Et was amidated by 3-(MeO)C6H4NH2 and the product cyclized to give, after ether hydrolysis, 7-hydroxy-4-phenyl-2-quinolinone which was etherified by 3-(4-methoxy-4-tetrahydropyranyl)benzyl chloride to give title compound II.

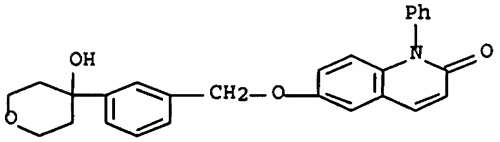
IT **167763-50-0P 167763-51-1P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heteroarylquinolines as leukotriene biosynthesis inhibitors)

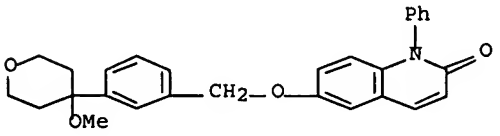
RN 167763-50-0 HCAPLUS

CN 2(1H)-Quinolinone, 1-phenyl-6-[[3-(tetrahydro-4-hydroxy-2H-pyran-4-yl)phenyl]methoxy]- (9CI) (CA INDEX NAME)



RN 167763-51-1 HCAPLUS

CN 2(1H)-Quinolinone, 1-phenyl-6-[[3-(tetrahydro-4-methoxy-2H-pyran-4-yl)phenyl]methoxy]- (9CI) (CA INDEX NAME)



L10 ANSWER 22 OF 22 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1988:112151 HCAPLUS Full-text

DOCUMENT NUMBER: 108:112151

TITLE: Action of nitrogen and carbon nucleophiles on 6-phenyl-3,4-dihydrocoumarin

AUTHOR(S): Sayed, M. A.; Soliman, A. Y.; El-Gendy, A. M.; Mostafa, M.

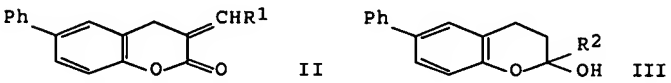
CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt

SOURCE: Oriental Journal of Chemistry (1987), 3(2), 174-8
CODEN: OJCHEG; ISSN: 0970-020X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



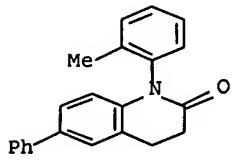
II III

AB The title coumarin (I) underwent a condensation reaction with aldehydes to give products II (R1 = Ph, 4-O2NC6H4, PhCH:CH, 2-HOC6H4); chromanols III (R3 = Et, anisyl, tolyl, Ph, cyclohexyl) were prepared from I, organic halides, and Mg. I and amines gave 3,4-dihydroquinolin-2(1H)-ones.

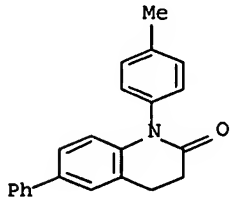
IT **113334-83-1P 113334-84-2P 113334-85-3P**
113334-87-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 113334-83-1 HCAPLUS

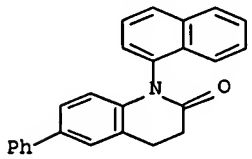
CN 2(1H)-Quinolinone, 3,4-dihydro-1-(2-methylphenyl)-6-phenyl- (9CI) (CA INDEX NAME)



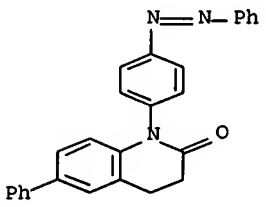
RN 113334-84-2 HCAPLUS
CN 2(1H)-Quinolinone, 3,4-dihydro-1-(4-methylphenyl)-6-phenyl- (9CI) (CA INDEX NAME)



RN 113334-85-3 HCAPLUS
CN 2(1H)-Quinolinone, 3,4-dihydro-1-(1-naphthalenyl)-6-phenyl- (9CI) (CA INDEX NAME)



RN 113334-87-5 HCAPLUS
CN 2(1H)-Quinolinone, 3,4-dihydro-6-phenyl-1-[4-(phenylazo)phenyl]- (9CI) (CA INDEX NAME)



=>
Connecting via Winsock to STN

```
Welcome to STN International!  Enter x:x

LOGINID:sspatrxs01

PASSWORD:
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 16:44:20 ON 16 APR 2007
FILE 'REGISTRY' ENTERED AT 16:44:20 ON 16 APR 2007
COPYRIGHT (C) 2007 American Chemical Society (ACS)

=> file reg
FILE 'REGISTRY' ENTERED AT 16:44:26 ON 16 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   15 APR 2007  HIGHEST RN 930272-82-5
DICTIONARY FILE UPDATES:  15 APR 2007  HIGHEST RN 930272-82-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
```